

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
 Data File : BF124113.D
 Acq On : 28 May 2021 18:41
 Operator : JU/CG
 Sample : M2539-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-073

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124113.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	14	rVB	464883	590448	82.08%	6.581%
2	2.246	24	27	32	rBV5	11012	15613	2.17%	0.174%
3	5.081	507	509	514	rVB	18313	20288	2.82%	0.226%
4	5.492	574	579	582	rBV	715043	662085	92.04%	7.380%
5	6.498	746	750	753	rBV	733182	610683	84.89%	6.807%
6	6.869	810	813	817	rBV	231704	196365	27.30%	2.189%
7	7.433	904	909	912	rBV	508400	438712	60.99%	4.890%
8	8.057	1011	1015	1023	rBV2	41630	51600	7.17%	0.575%
9	8.157	1028	1032	1035	rVB	244674	215017	29.89%	2.397%
10	9.227	1211	1214	1218	rBV	833376	664134	92.32%	7.402%
11	9.910	1327	1330	1333	rBV	305534	234007	32.53%	2.608%
12	10.698	1460	1464	1468	rBV	600395	466507	64.85%	5.200%
13	10.810	1481	1483	1489	rBV2	10874	13585	1.89%	0.151%
14	11.398	1580	1583	1586	rBV	298030	231788	32.22%	2.584%
15	11.451	1590	1592	1594	rVB2	13064	9207	1.28%	0.103%
16	11.921	1670	1672	1683	rBV5	23912	24891	3.46%	0.277%
17	12.657	1794	1797	1801	rVB	36248	33335	4.63%	0.372%
18	12.986	1849	1853	1856	rBV	887556	719364	100.00%	8.018%
19	13.215	1890	1892	1897	rBV4	12213	16233	2.26%	0.181%
20	13.368	1915	1918	1919	rBV3	12203	10064	1.40%	0.112%
21	13.386	1919	1921	1924	rVV4	13852	16719	2.32%	0.186%
22	13.427	1924	1928	1932	rVV7	14929	28541	3.97%	0.318%
23	13.492	1937	1939	1943	rVB4	31187	29801	4.14%	0.332%
24	13.557	1945	1950	1952	rBV5	34385	44101	6.13%	0.492%
25	13.645	1953	1965	1966	rBV7	109836	276990	38.50%	3.087%
26	13.892	2002	2007	2008	rBV2	40330	51635	7.18%	0.576%
27	13.910	2008	2010	2017	rVV3	84735	121307	16.86%	1.352%
28	13.968	2019	2020	2025	rVV4	15826	13455	1.87%	0.150%
29	14.039	2029	2032	2036	rVV	290004	273887	38.07%	3.053%
30	14.204	2055	2060	2064	rBV	44179	54177	7.53%	0.604%
31	14.445	2099	2101	2104	rVB4	10758	10697	1.49%	0.119%
32	14.509	2109	2112	2115	rVV	70661	72691	10.10%	0.810%
33	14.557	2115	2120	2127	rVV9	37501	94553	13.14%	1.054%
34	14.645	2131	2135	2136	rVB4	13350	15530	2.16%	0.173%
35	14.821	2161	2165	2171	rVB	55759	65421	9.09%	0.729%
36	14.898	2176	2178	2183	rVB5	22980	26319	3.66%	0.293%

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 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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37	14.974	2188	2191	2196	rVB5	20270	24276	3.37%	0.271%
38	15.051	2201	2204	2207	rBV5	10087	11958	1.66%	0.133%
39	15.086	2207	2210	2211	rBV3	10812	11262	1.57%	0.126%
40	15.168	2220	2224	2229	rBV	148978	160846	22.36%	1.793%
41	15.339	2250	2253	2259	rVB7	17478	27096	3.77%	0.302%
42	15.451	2268	2272	2273	rBV4	10830	13682	1.90%	0.152%
43	15.527	2280	2285	2289	rBV	253682	334461	46.49%	3.728%
44	15.762	2320	2325	2331	rBV6	44564	67870	9.43%	0.756%
45	15.904	2346	2349	2355	rVB6	15050	25992	3.61%	0.290%
46	16.003	2362	2366	2372	rVB2	80510	120086	16.69%	1.338%
47	16.086	2375	2380	2381	rBV5	38169	59974	8.34%	0.668%
48	16.245	2404	2407	2408	rBV3	11990	12568	1.75%	0.140%
49	16.439	2437	2440	2441	rBV2	11233	11026	1.53%	0.123%
50	16.480	2446	2447	2450	rVV3	10649	9864	1.37%	0.110%
51	16.521	2452	2454	2458	rVB5	24129	31262	4.35%	0.348%
52	16.680	2478	2481	2482	rBV3	9316	9369	1.30%	0.104%
53	16.821	2500	2505	2516	rBV9	37878	74107	10.30%	0.826%
54	17.062	2543	2546	2548	rBV3	14756	19563	2.72%	0.218%
55	17.127	2555	2557	2564	rVB7	24027	46997	6.53%	0.524%
56	17.274	2578	2582	2583	rBV4	11889	13646	1.90%	0.152%
57	17.303	2583	2587	2588	rVV4	17276	22360	3.11%	0.249%
58	17.333	2588	2592	2603	rVB4	43111	112602	15.65%	1.255%
59	17.674	2643	2650	2655	rBV9	93653	284909	39.61%	3.176%
60	17.803	2668	2672	2674	rBV4	19391	29404	4.09%	0.328%
61	17.850	2677	2680	2687	rVB7	39578	81202	11.29%	0.905%
62	18.027	2702	2710	2711	rBV7	33650	63481	8.82%	0.708%
63	18.133	2725	2728	2730	rBV4	20734	23259	3.23%	0.259%
64	18.156	2730	2732	2734	rVV3	26029	30096	4.18%	0.335%
65	18.209	2734	2741	2754	rVB3	119183	344398	47.88%	3.839%
66	18.533	2782	2796	2797	rBV3	56698	158174	21.99%	1.763%
67	18.680	2813	2821	2838	rVB3	86814	316311	43.97%	3.526%

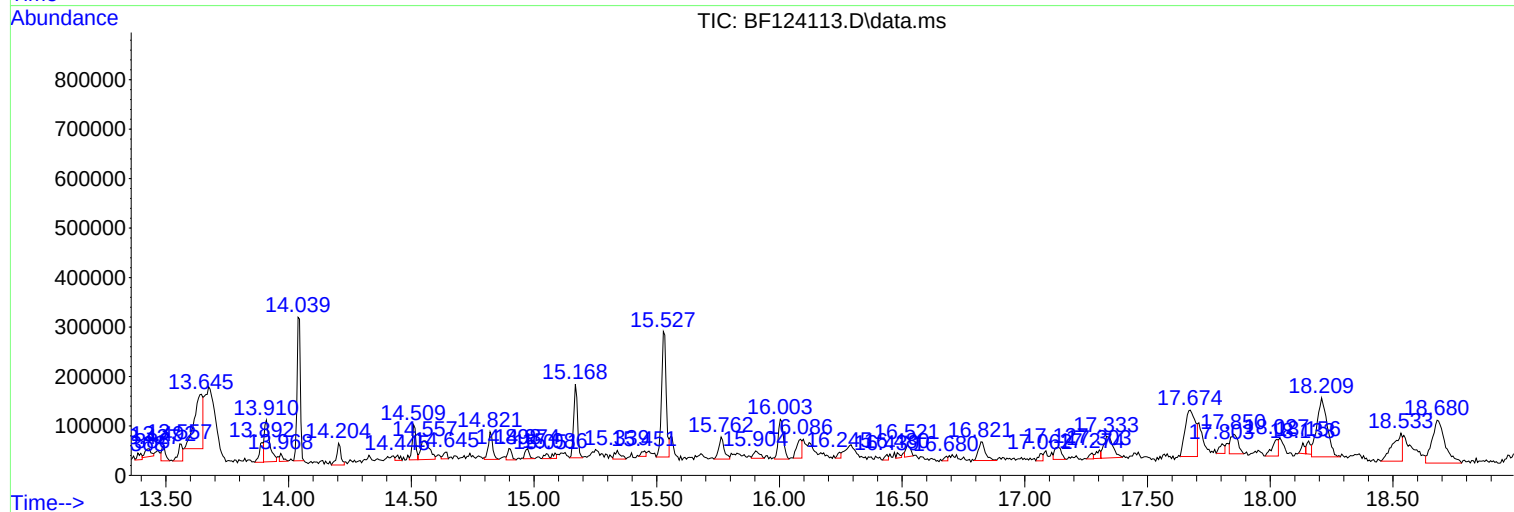
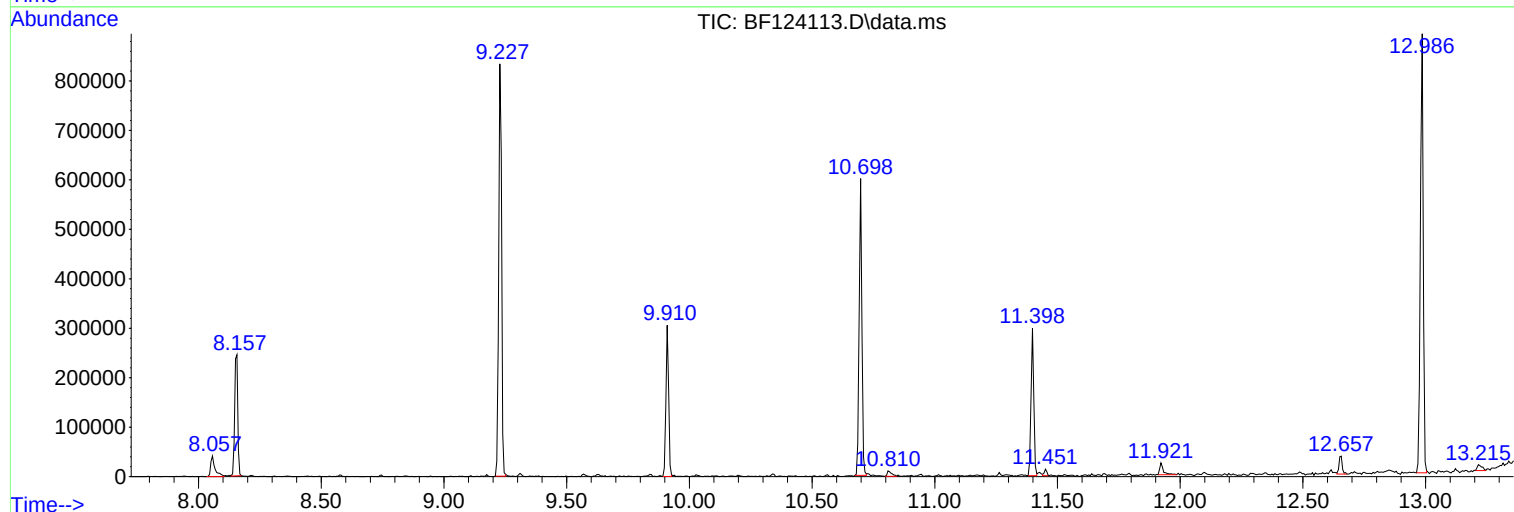
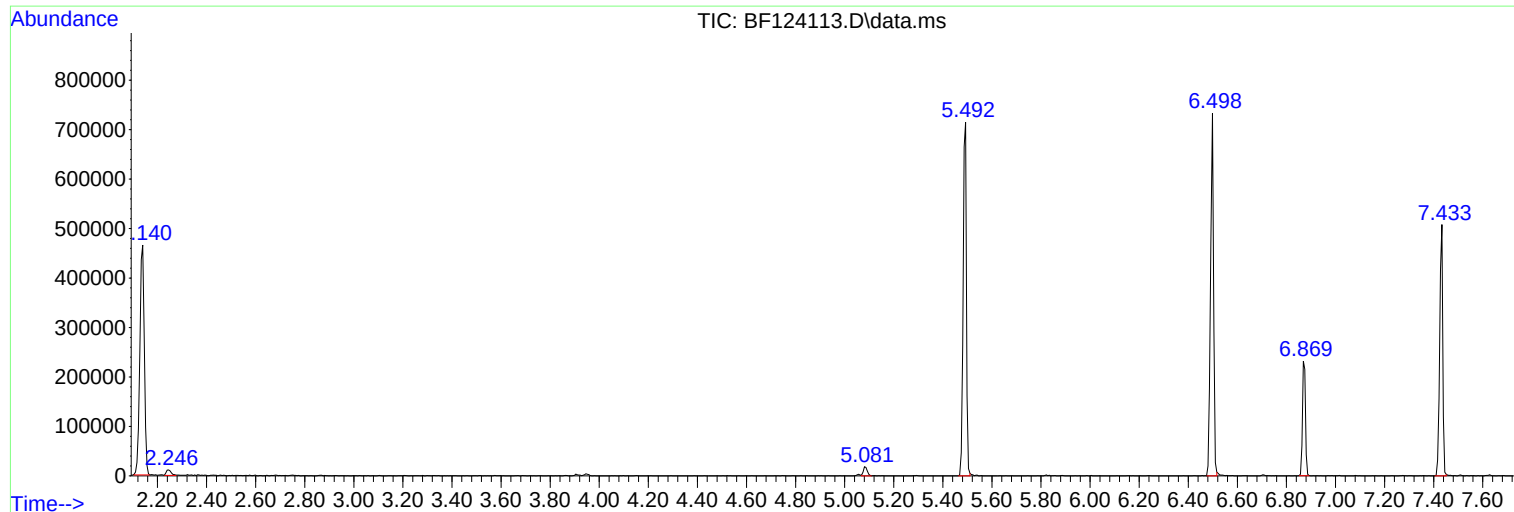
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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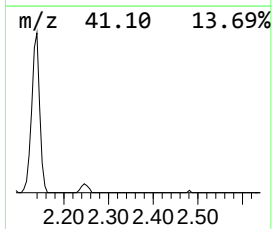
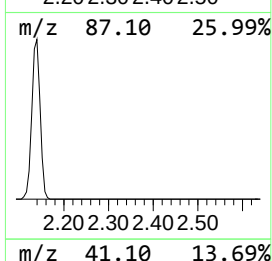
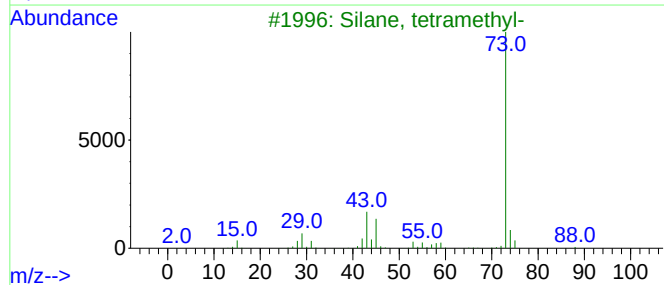
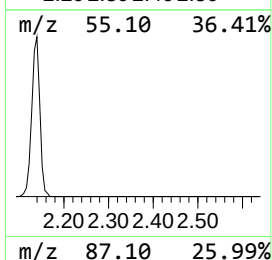
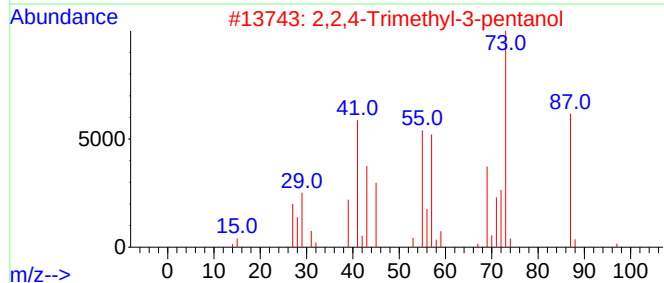
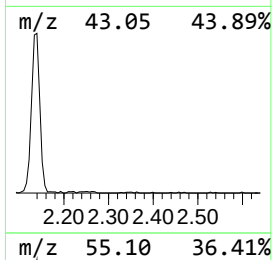
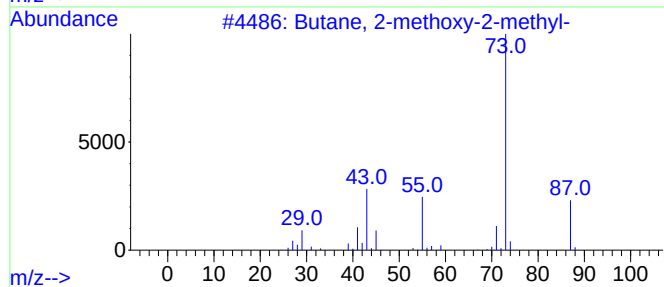
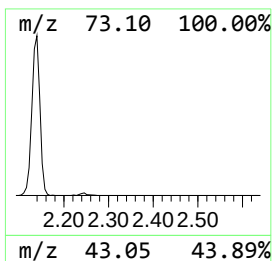
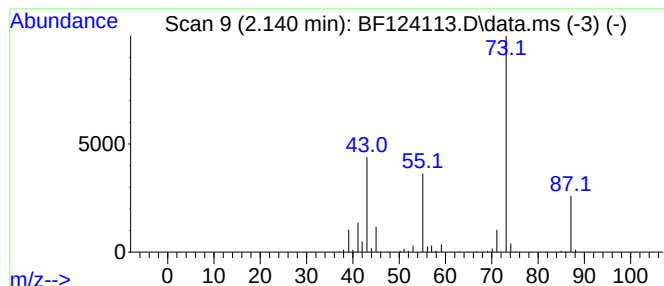
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	60.14 ng	590448	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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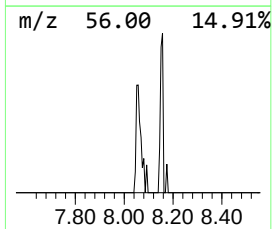
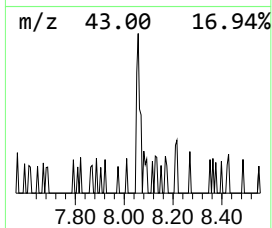
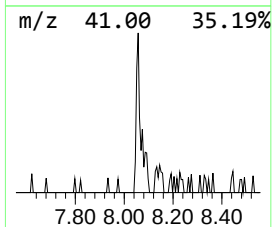
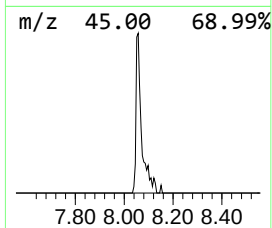
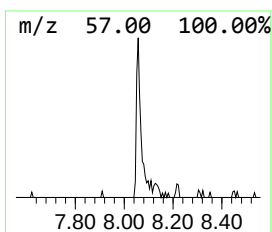
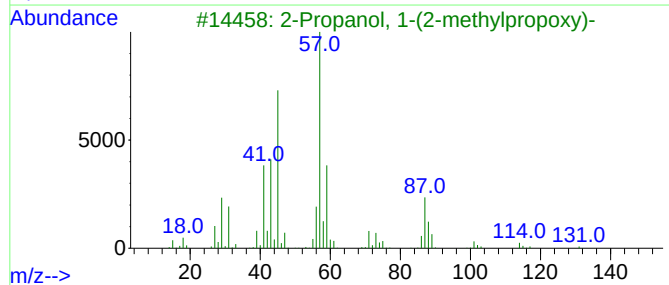
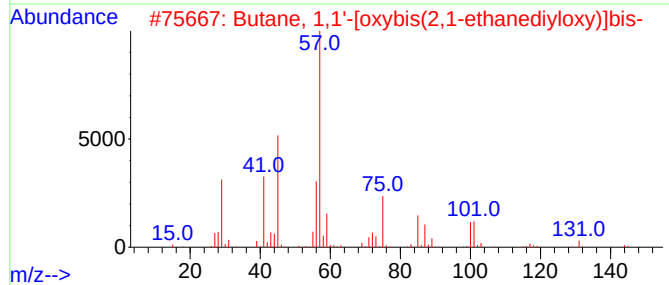
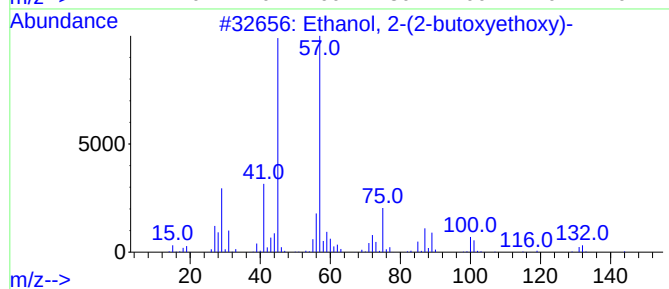
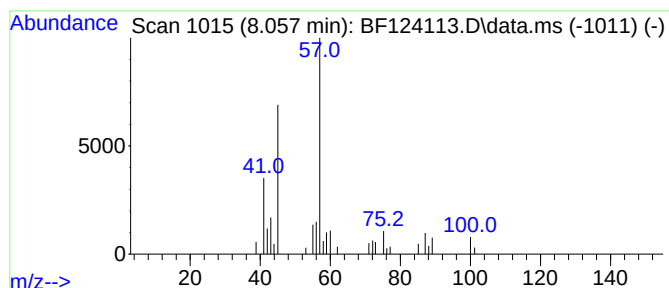
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.057	4.80 ng	51600	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
2			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	50
3			2-Propanol, 1-(2-methylpropoxy)-	132	C7H16O2	023436-19-3	40
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	40
5			Ethane, 1-methoxy-2-(methoxymeth...	120	C5H12O3	074498-88-7	38



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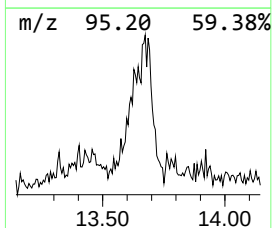
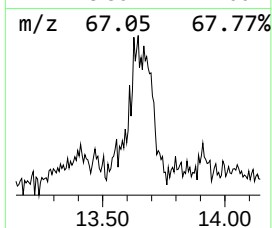
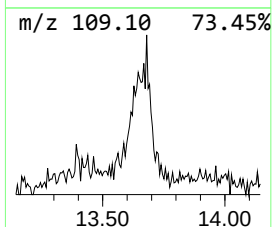
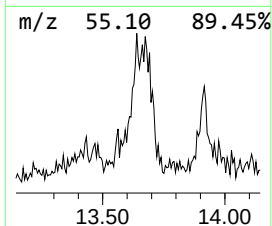
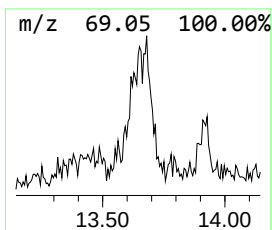
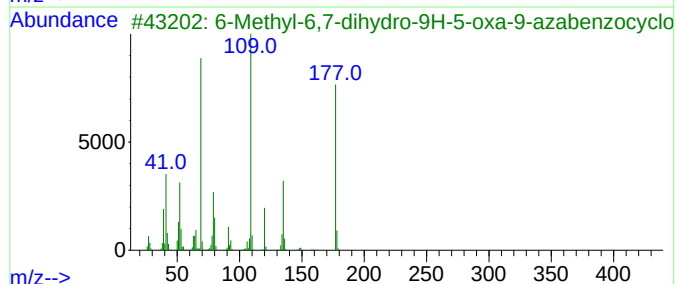
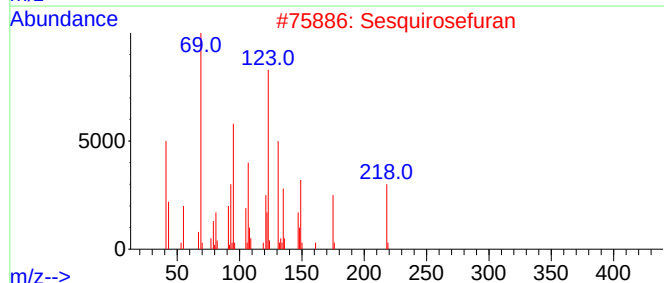
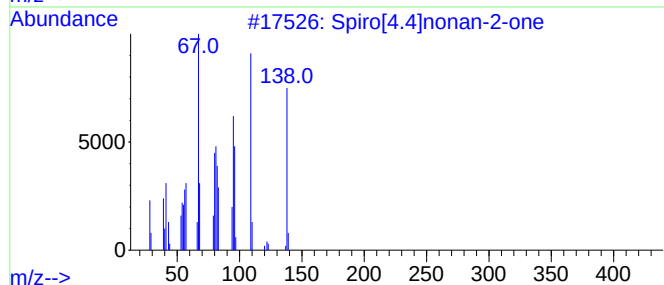
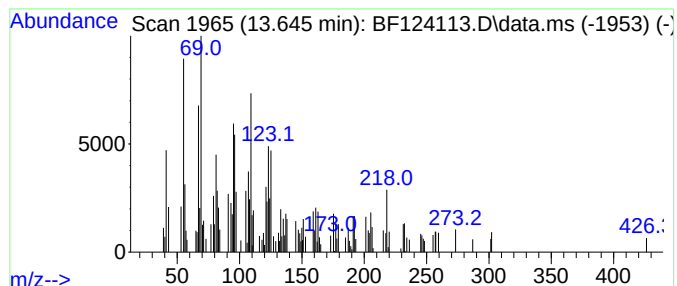
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown13.645 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.645	20.23 ng	276990	Chrysene-d12		14.045	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Spiro[4.4]nonan-2-one		138	C9H14O	034177-18-9	42
2	Sesquirosefuran		218	C15H22O	039007-93-7	41
3	6-Methyl-6,7-dihydro-9H-5-oxa-9-...		177	C10H11NO2	1000210-20-2	41
4	2H-1,6-Benzoxazocin-5(6H)-one, 3...		177	C10H11NO2	051110-93-1	38
5	1-Formyl-2,2,6-trimethyl-3-cis-(...		220	C15H24O	1000144-10-1	38



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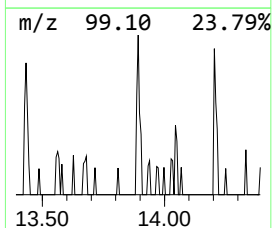
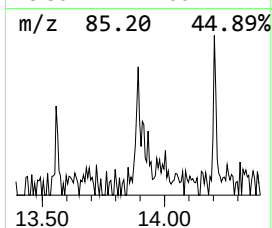
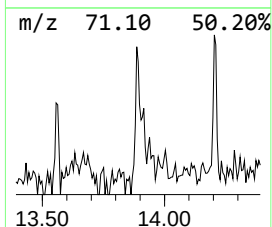
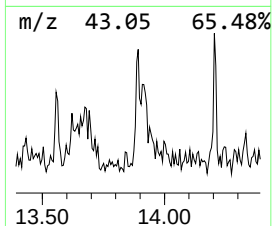
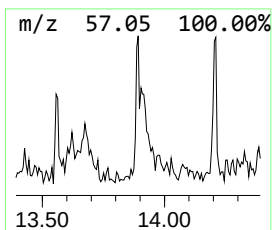
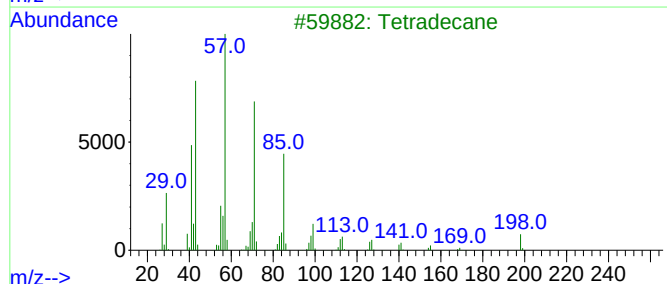
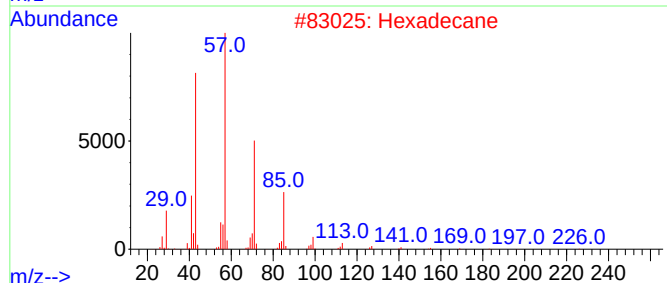
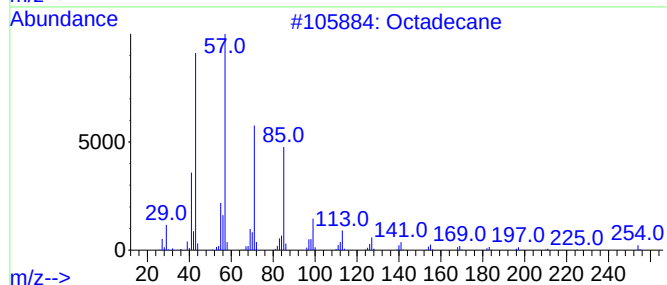
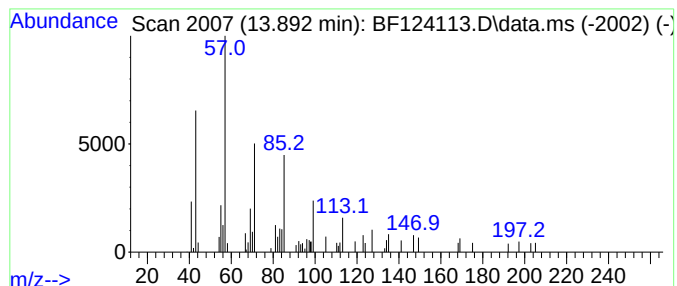
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.77 ng	51635	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	72
2			Hexadecane	226	C16H34	000544-76-3	72
3			Tetradecane	198	C14H30	000629-59-4	72
4			Heneicosane	296	C21H44	000629-94-7	72
5			Hentriacontane	437	C31H64	000630-04-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
Acq On : 28 May 2021 18:41
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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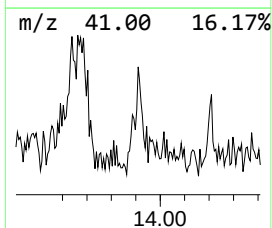
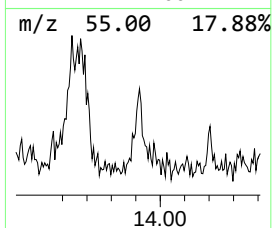
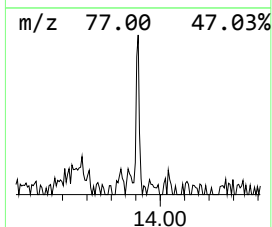
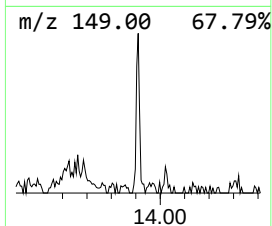
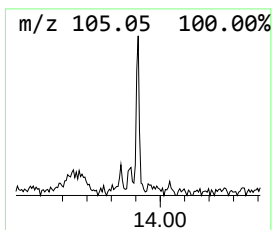
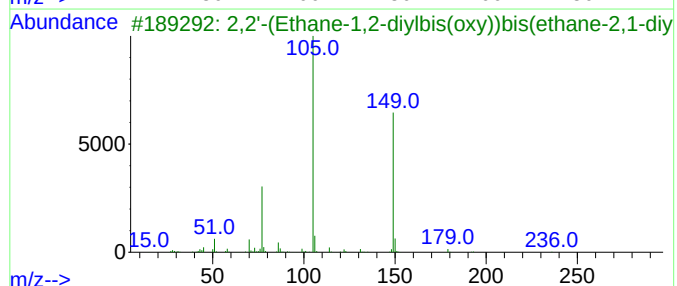
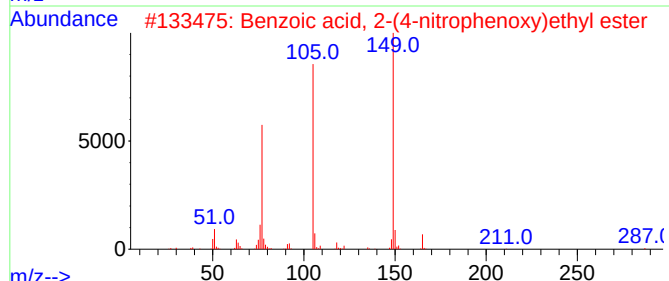
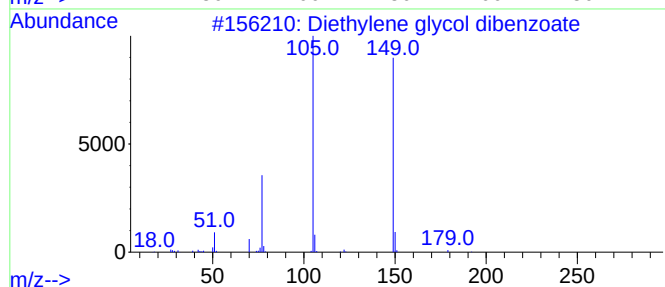
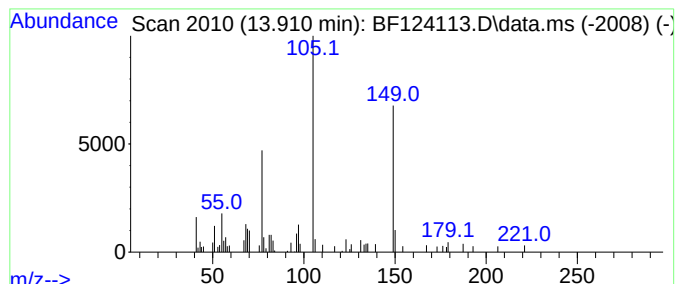
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	8.86 ng	121307	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	59
2			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	53
3			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	45
4			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	45
5			2-(2-(2-Butoxyethoxy)ethoxy)ethy...	310	C17H26O5	1000366-97-2	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
Acq On : 28 May 2021 18:41
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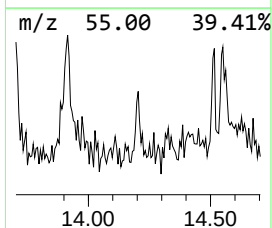
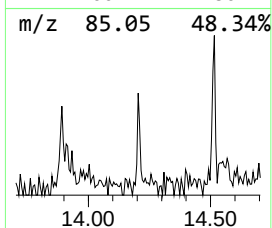
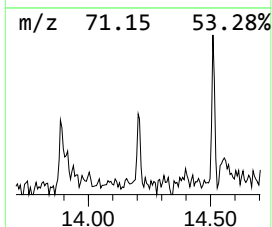
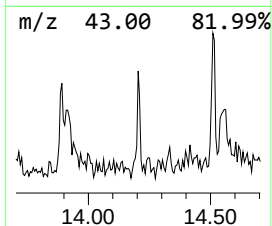
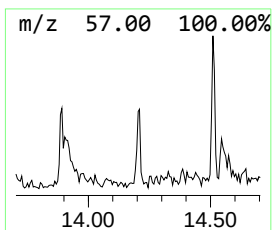
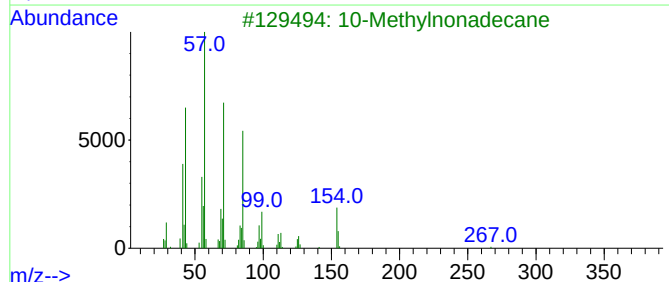
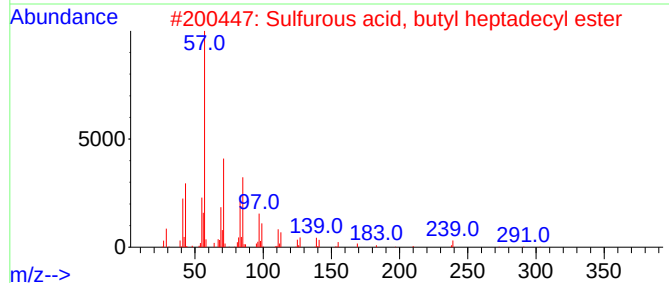
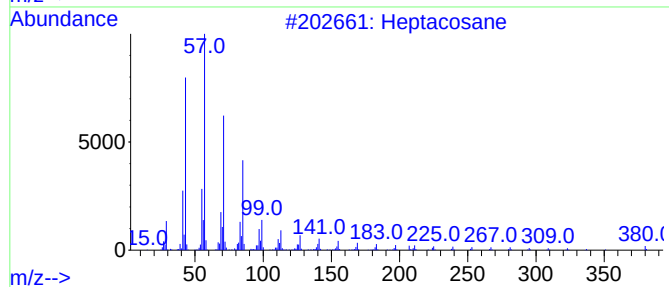
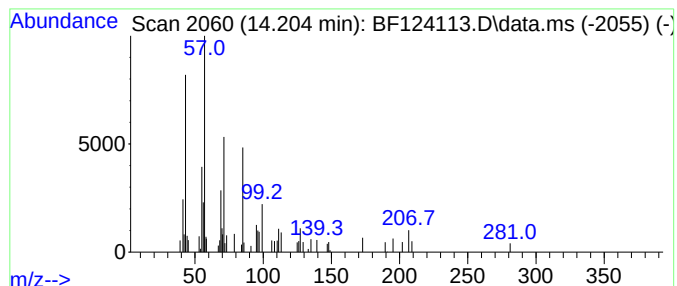
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptacosane Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.204	3.96 ng	54177	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	59
2			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	59
3			10-Methylnonadecane	282	C20H42	056862-62-5	59
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	53
5			2-Bromotetradecane	276	C14H29Br	074036-95-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
Acq On : 28 May 2021 18:41
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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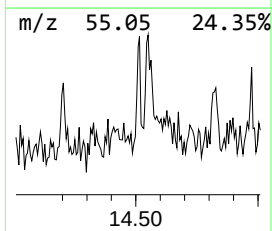
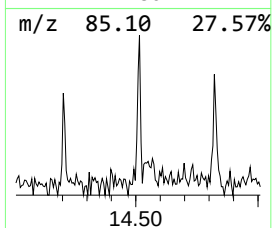
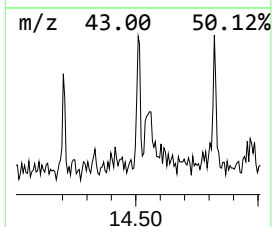
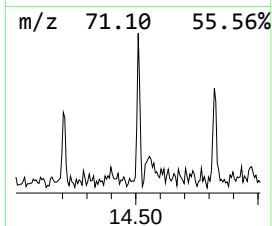
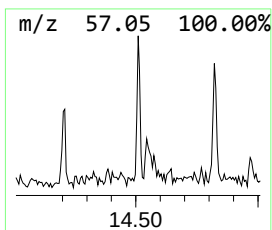
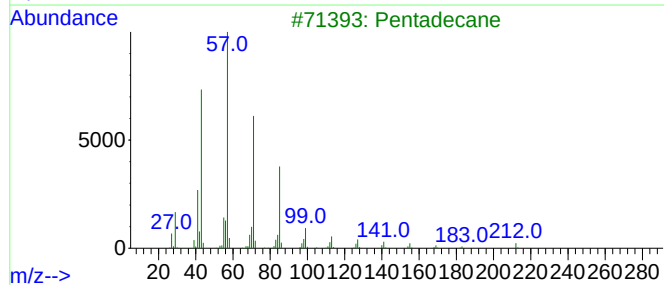
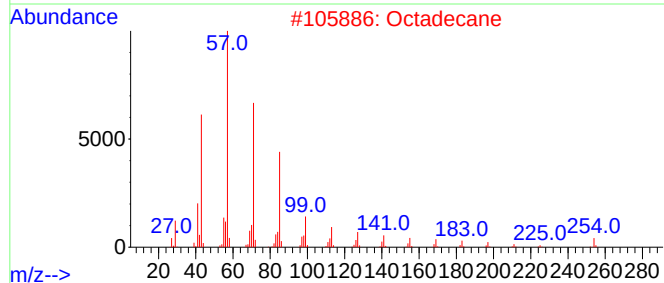
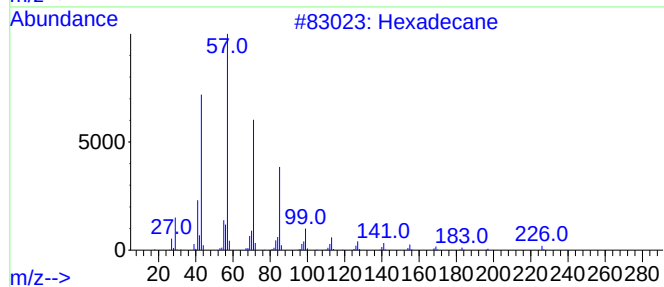
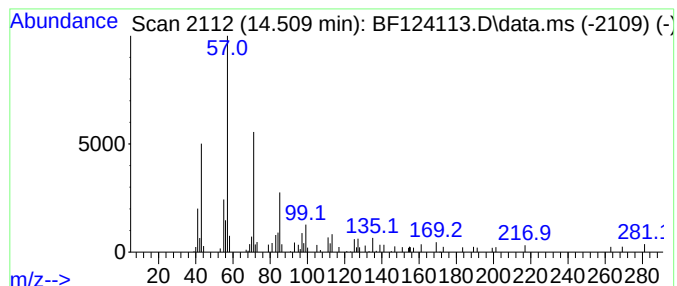
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.509	5.31 ng	72691	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	80
2			Octadecane	254	C18H38	000593-45-3	72
3			Pentadecane	212	C15H32	000629-62-9	64
4			Tetracosane	338	C24H50	000646-31-1	64
5			Heptadecane	240	C17H36	000629-78-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
Acq On : 28 May 2021 18:41
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Sample : M2539-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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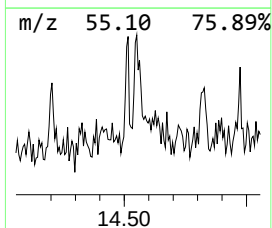
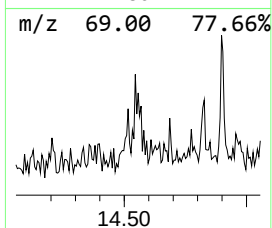
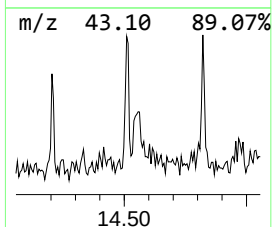
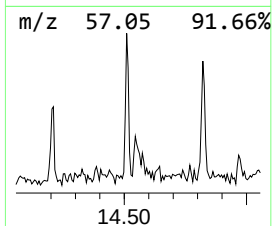
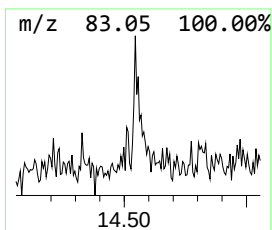
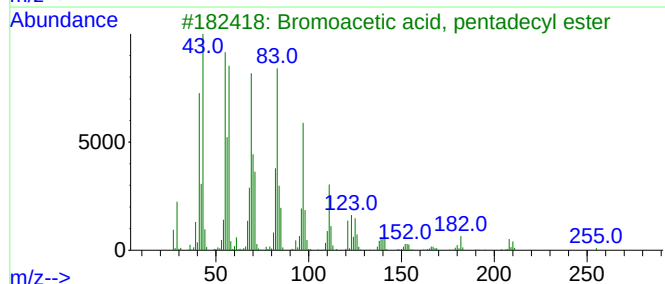
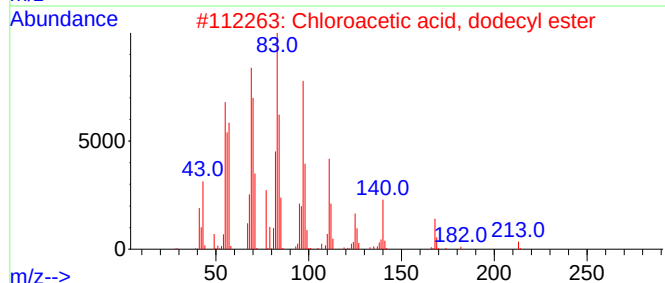
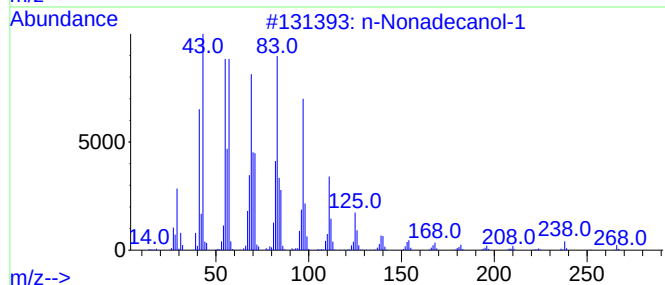
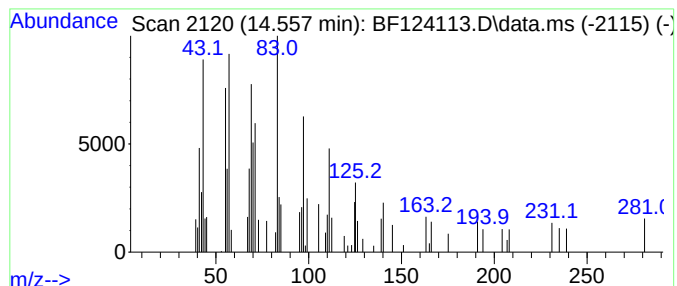
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 n-Nonadecanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	6.90 ng	94553	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	64
2			Chloroacetic acid, dodecyl ester	262	C14H27ClO2	006316-04-7	58
3			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	58
4			1-Octadecanol	270	C18H38O	000112-92-5	52
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
Acq On : 28 May 2021 18:41
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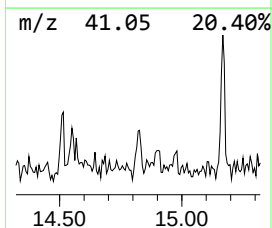
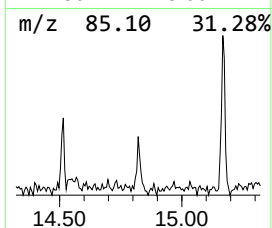
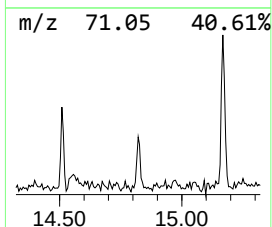
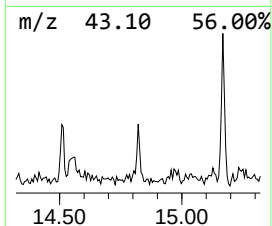
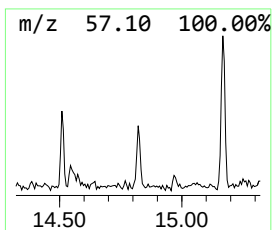
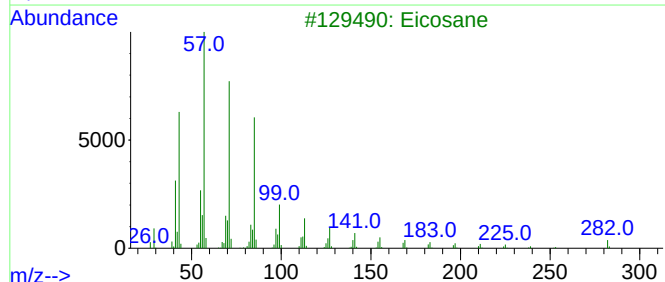
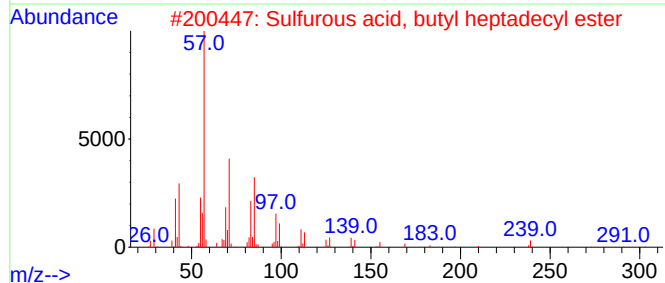
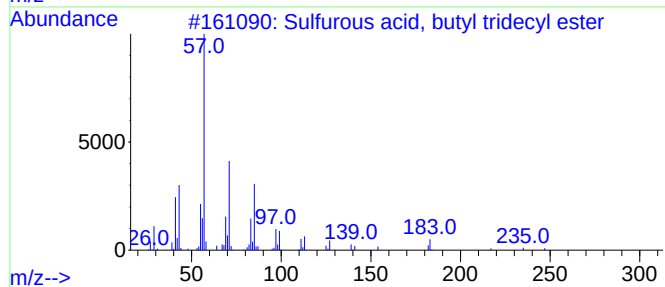
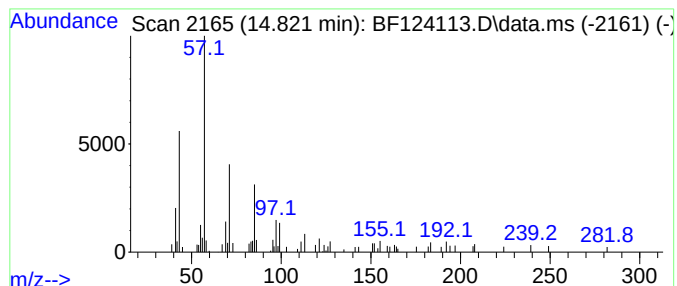
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Sulfurous acid, butyl tridecyl... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	3.91 ng	65421	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	80
2			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	80
3			Eicosane	282	C20H42	000112-95-8	76
4			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	72
5			Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
Acq On : 28 May 2021 18:41
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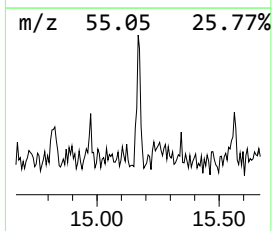
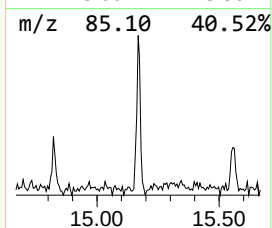
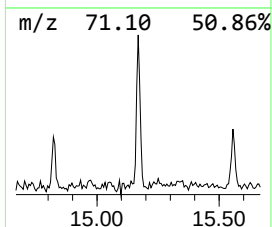
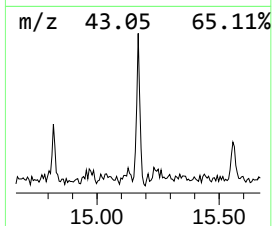
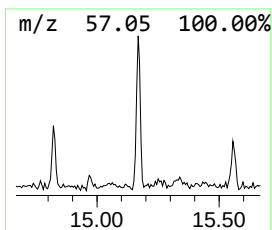
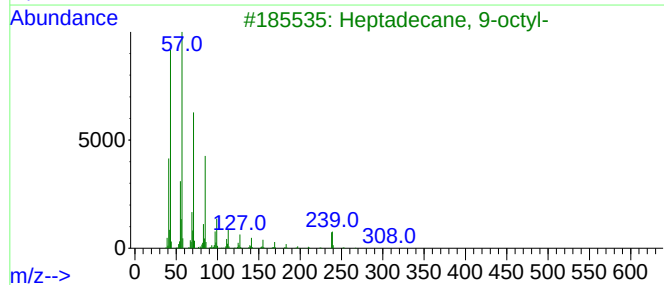
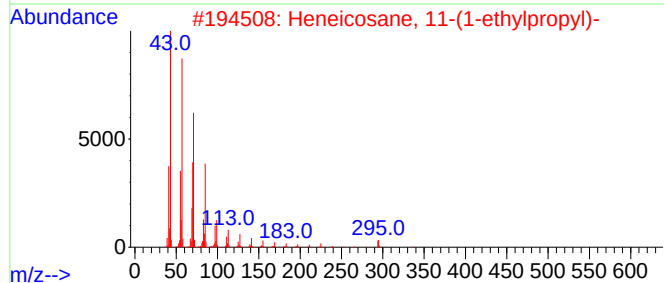
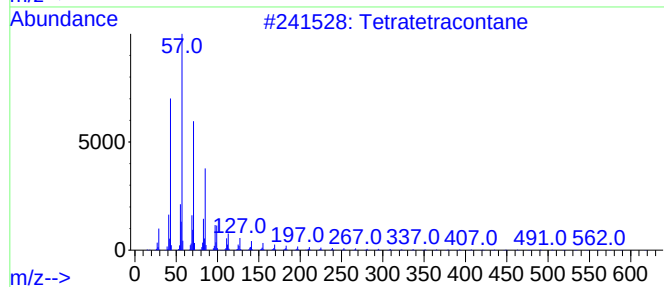
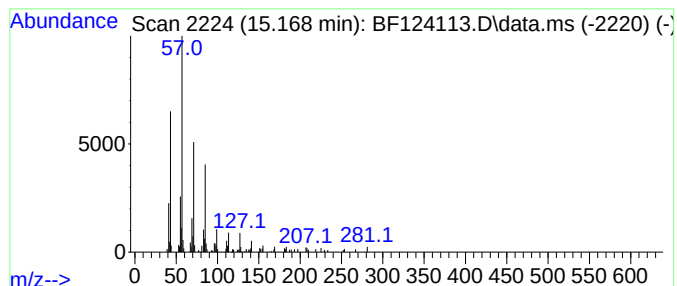
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.168	9.62 ng	160846	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Octacosane	394	C28H58	000630-02-4	90
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
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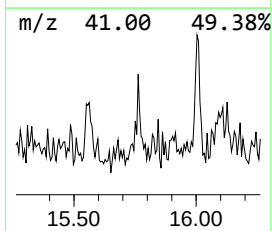
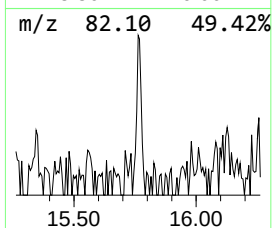
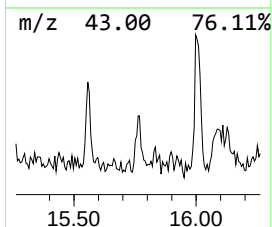
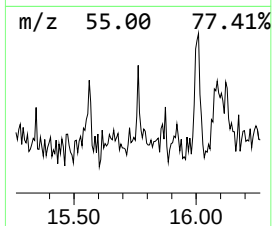
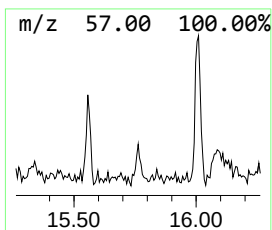
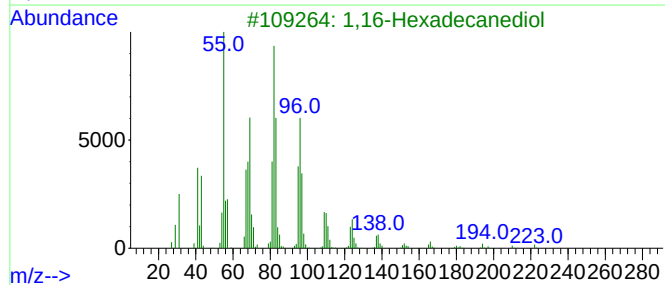
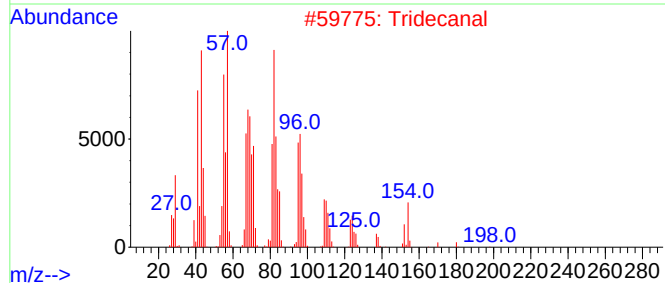
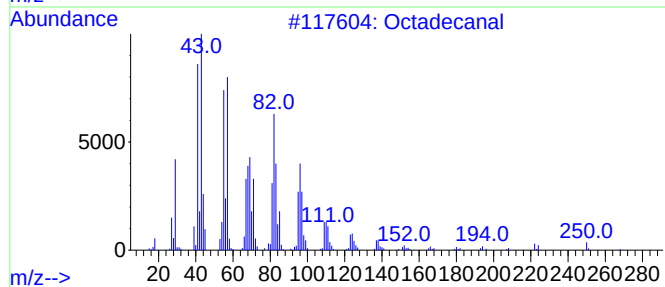
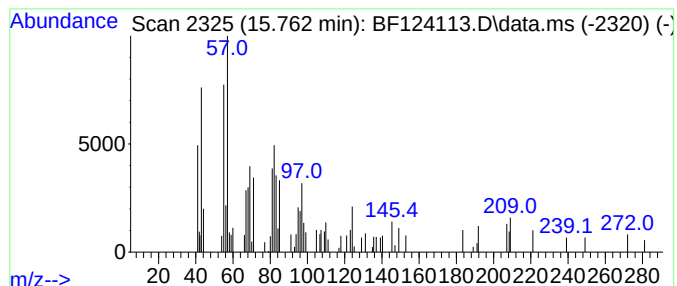
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown15.762 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.762	4.06 ng	67870	Perylene-d12	15.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanal	268	C18H36O	000638-66-4	46
2		Tridecanal	198	C13H26O	010486-19-8	38
3		1,16-Hexadecanediol	258	C16H34O2	007735-42-4	38
4		trans-2-Dodecen-1-ol	184	C12H24O	069064-37-5	35
5		Z,Z-3,13-Octadecadien-1-ol	266	C18H34O	1000131-10-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
Acq On : 28 May 2021 18:41
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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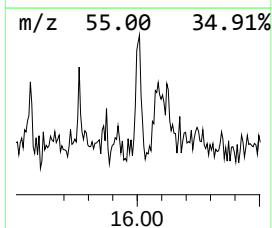
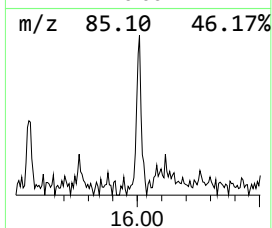
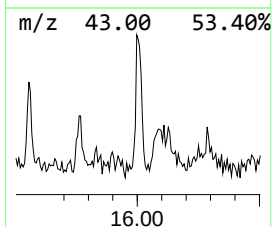
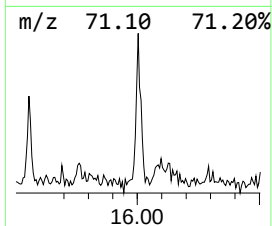
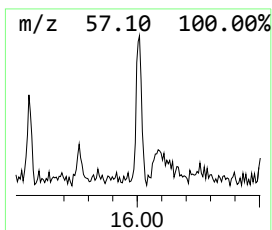
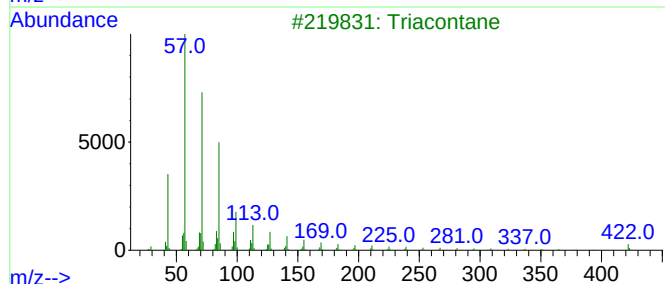
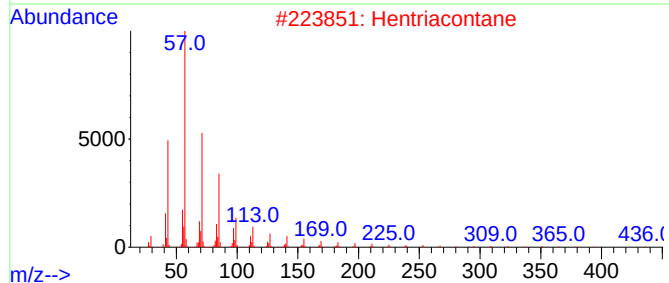
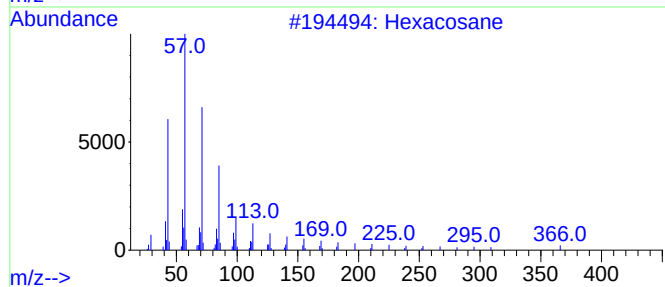
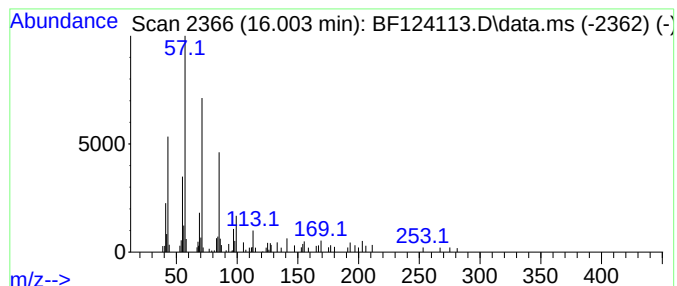
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.003	7.18 ng	120086	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	86
2			Hentriacontane	437	C31H64	000630-04-6	86
3			Triacontane	422	C30H62	000638-68-6	86
4			Docosane	310	C22H46	000629-97-0	80
5			Octadecane	254	C18H38	000593-45-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
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ClientSampleId :
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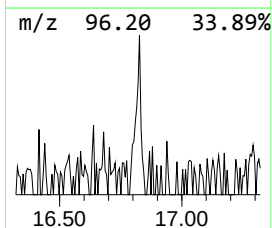
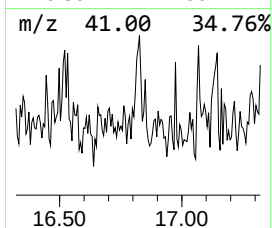
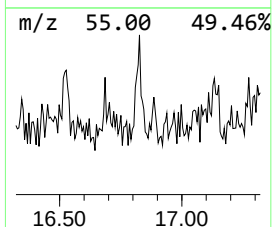
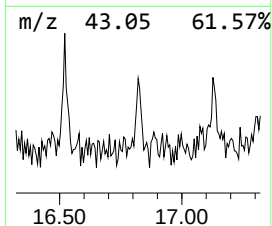
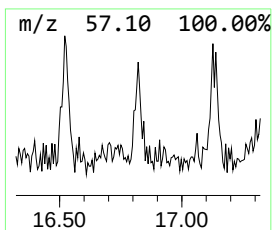
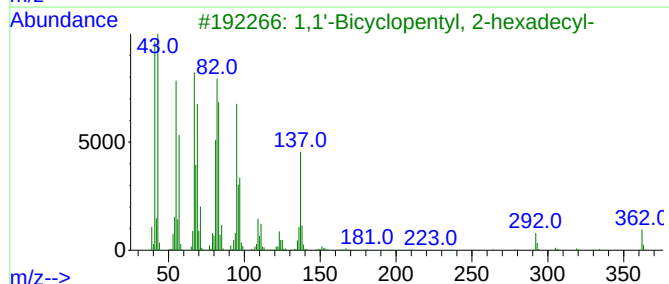
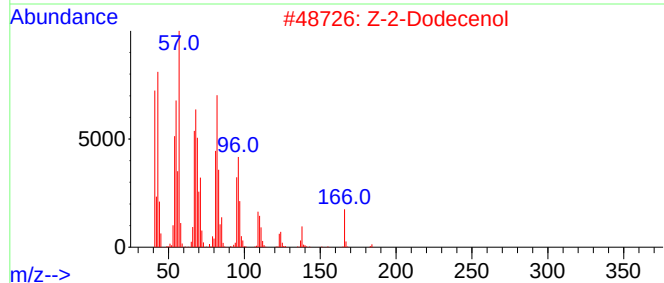
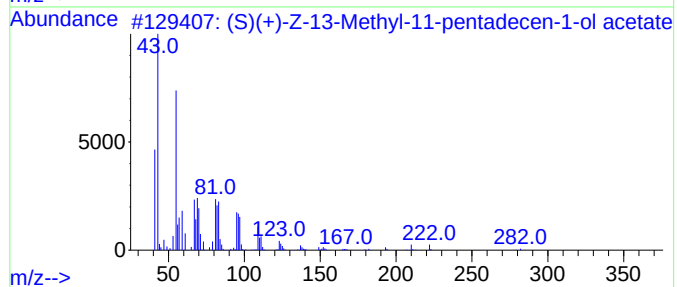
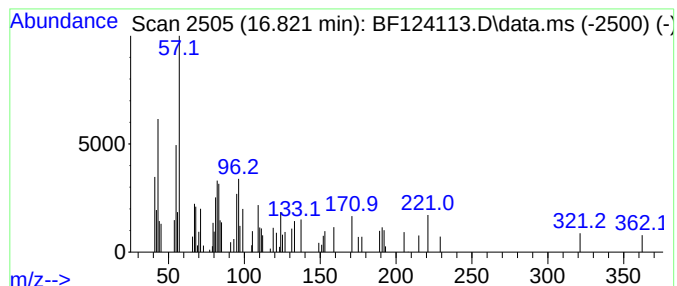
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown16.821 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.821	4.43 ng	74107	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)(+)-Z-13-Methyl-11-pentadecen...	282	C18H34O2	1000130-84-8	35		
2	Z-2-Dodecenol	184	C12H24O	069064-36-4	22		
3	1,1'-Bicyclopentyl, 2-hexadecyl-	362	C26H50	055334-11-7	20		
4	2-Decen-1-ol, (E)-	156	C10H20O	018409-18-2	14		
5	trans-2-Dodecen-1-ol	184	C12H24O	069064-37-5	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
Acq On : 28 May 2021 18:41
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
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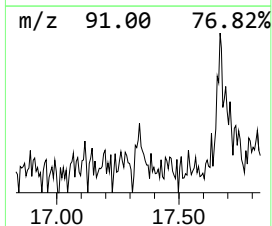
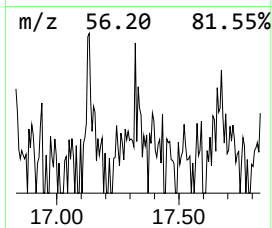
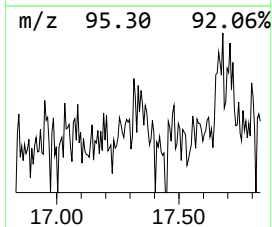
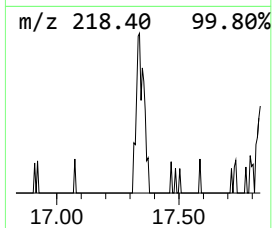
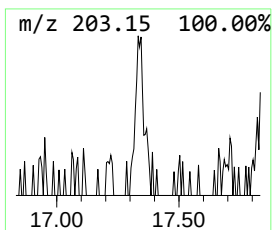
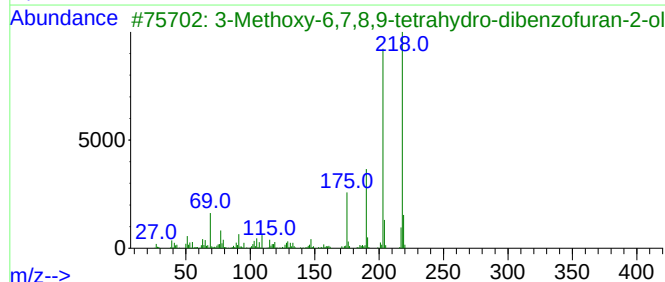
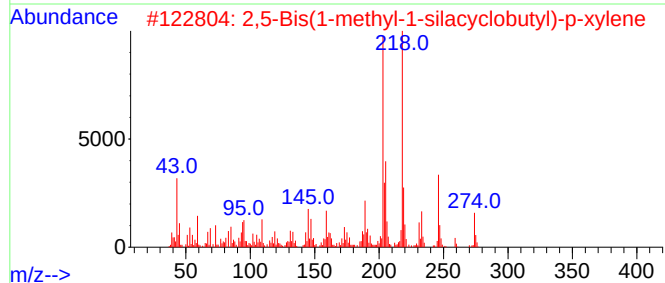
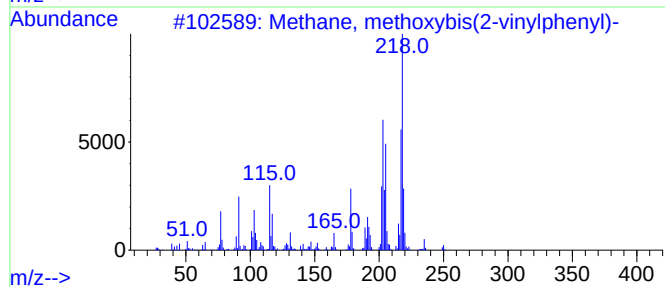
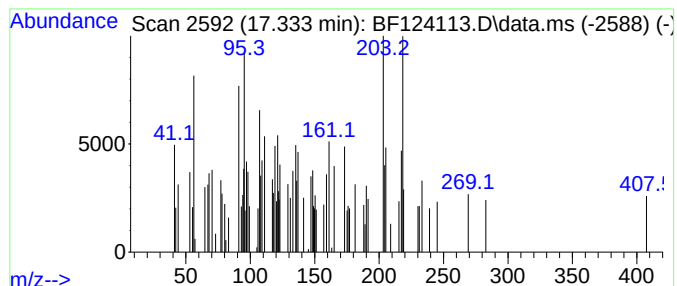
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown17.333 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.333	6.73 ng	112602	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, methoxybis(2-vinylphenyl)-	250	C18H18O	1000210-69-5	38
2			2,5-Bis(1-methyl-1-silacyclobuty...	274	C16H26Si2	1000280-74-9	37
3			3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	27
4			6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	25
5			2,10-Dimethyl-2,3,4,5,6,7-hexahy...	203	C14H21N	077581-13-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
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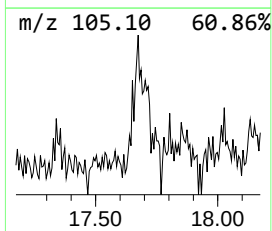
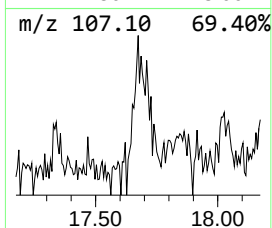
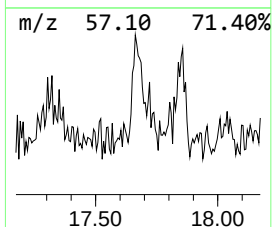
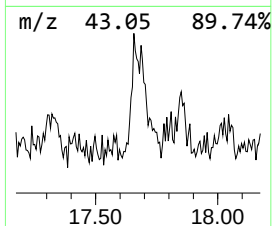
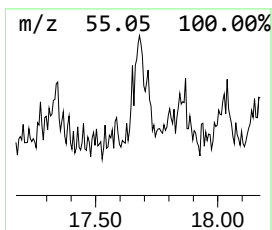
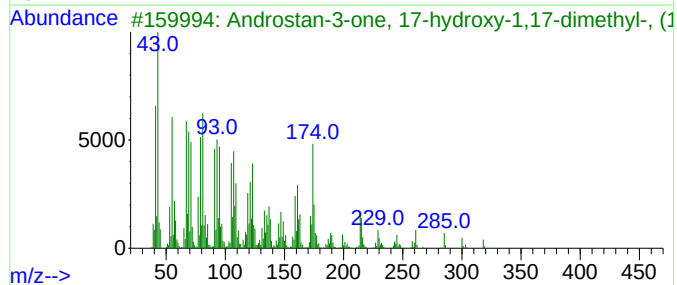
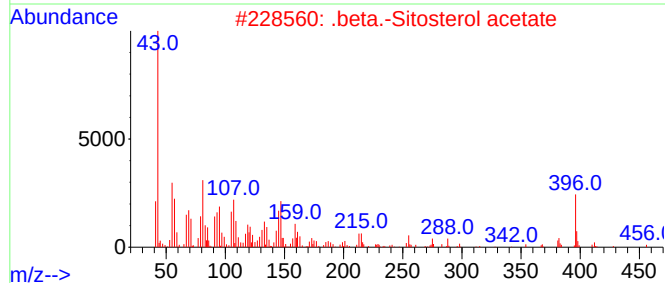
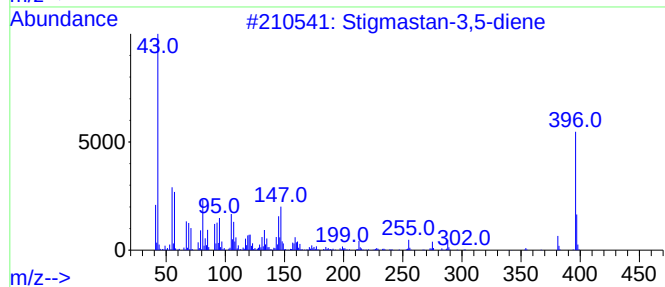
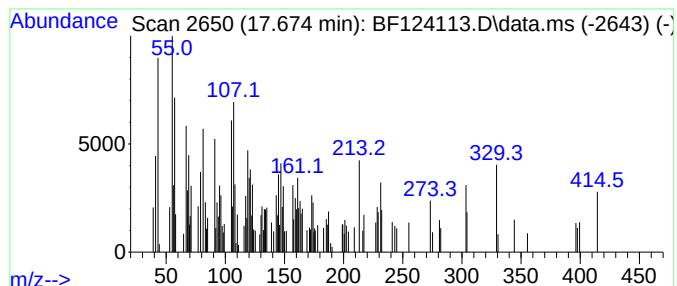
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown17.674 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.674	17.04 ng	284909	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Stigmastan-3,5-diene	396	C29H48	1000214-16-4	25
2			.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	10
3			Androstan-3-one, 17-hydroxy-1,17...	318	C21H34O2	002881-21-2	10
4			Pregn-4-ene-3,20-dione, dioxime	344	C21H32N2O2	026144-38-7	9
5			Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
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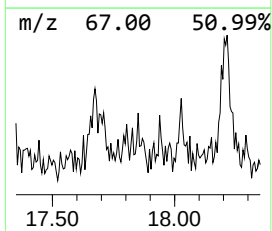
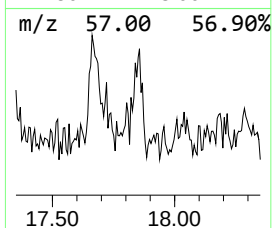
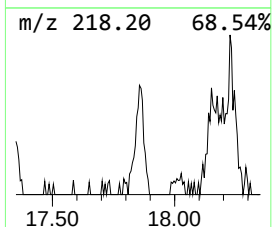
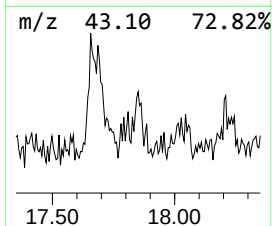
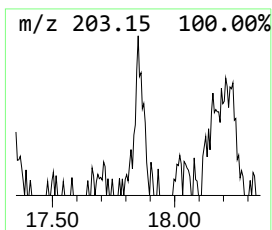
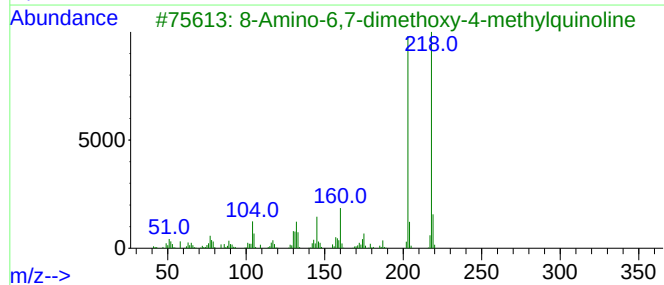
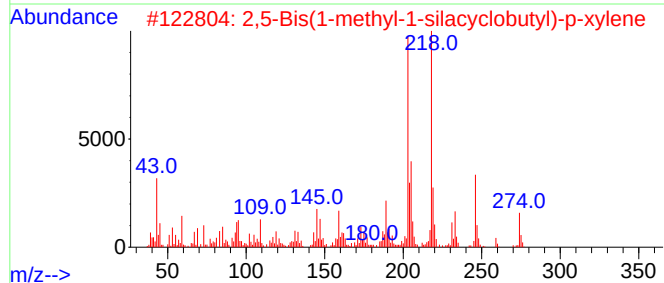
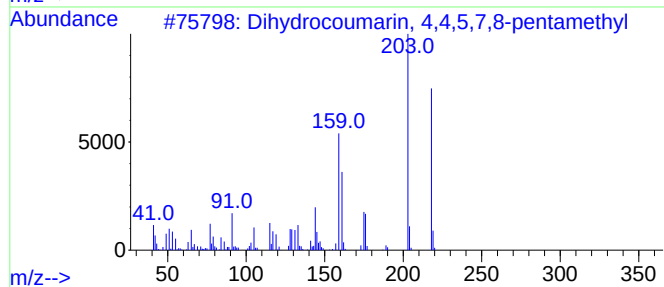
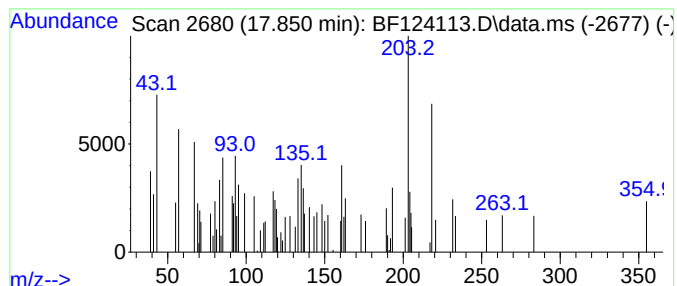
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 unknown17.850 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.850	4.86 ng	81202	Perylene-d12	15.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dihydrocoumarin, 4,4,5,7,8-penta...	218	C14H18O2	039170-97-3	43
2		2,5-Bis(1-methyl-1-silacyclobuty...	274	C16H26Si2	1000280-74-9	35
3		8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	27
4		3-Acethyl-6-methoxycoumarine	218	C12H10O4	013252-80-7	27
5		9,11-Dimethyltetracyclo[7.3.1.0(...	218	C16H26	053263-99-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
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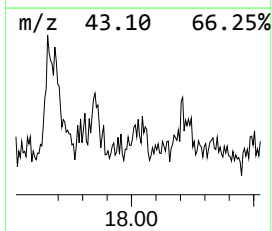
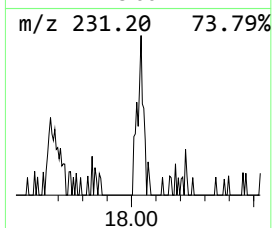
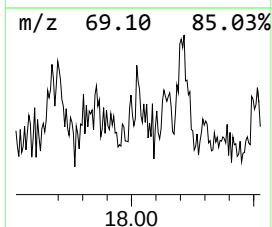
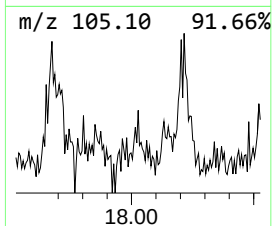
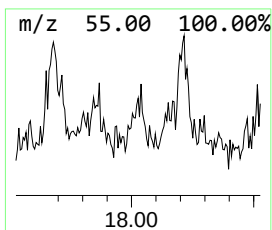
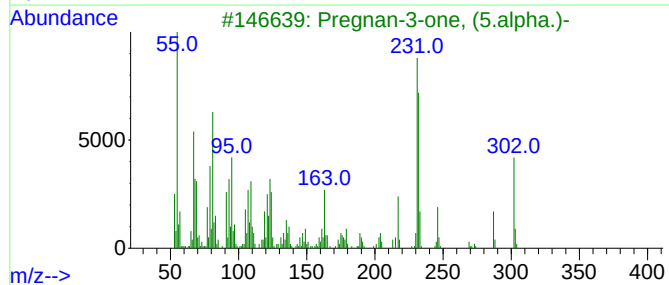
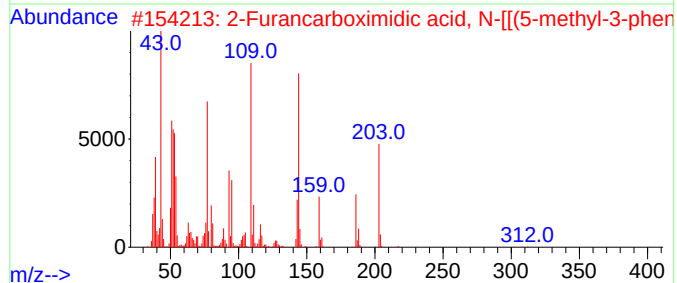
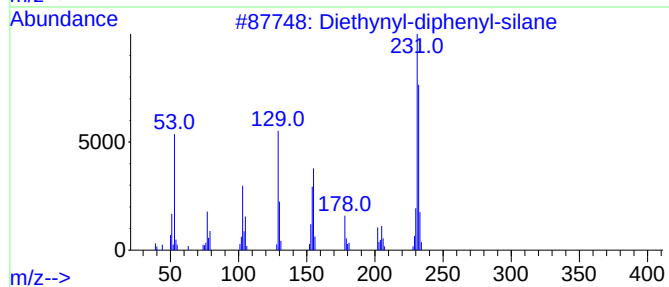
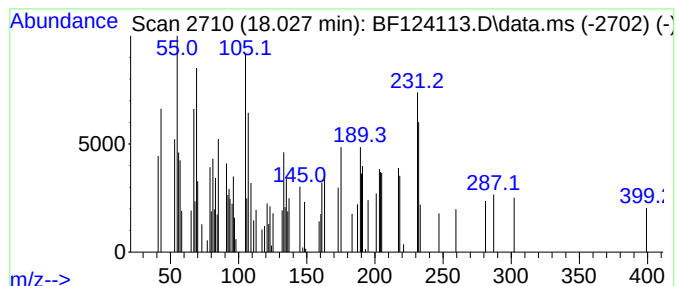
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 unknown18.027 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.027	3.80 ng	63481	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethynyl-diphenyl-silane	232	C16H12Si	001675-57-6	38
2			2-Furancarboximide acid, N-[(5-methyl-3-phenyl)-	312	C16H12N2O5	1000316-35-1	27
3			Pregnan-3-one, (5.alpha.)-	302	C21H34O	014778-11-1	16
4			Phenol, 2-amino-4-(3-amino-4-hydroxyphenyl)-	232	C12H12N2O3	1000327-59-3	16
5			Toluene,3-cyclopropylmethoxy	162	C11H14O	1000222-96-8	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
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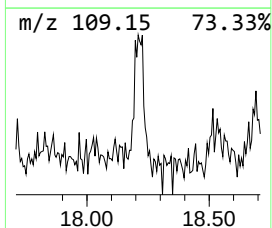
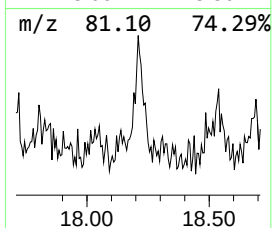
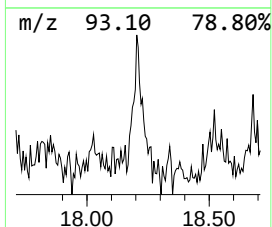
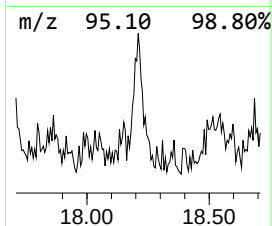
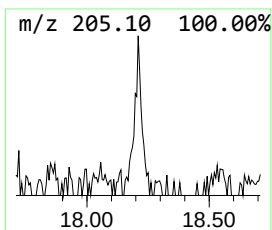
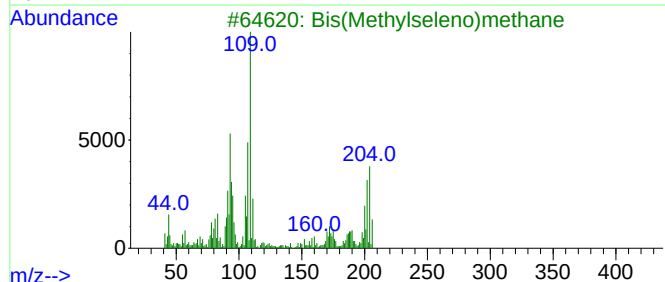
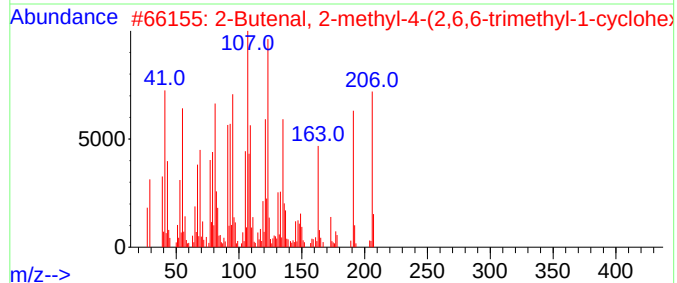
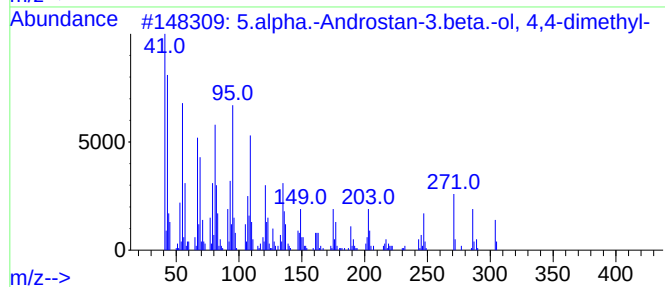
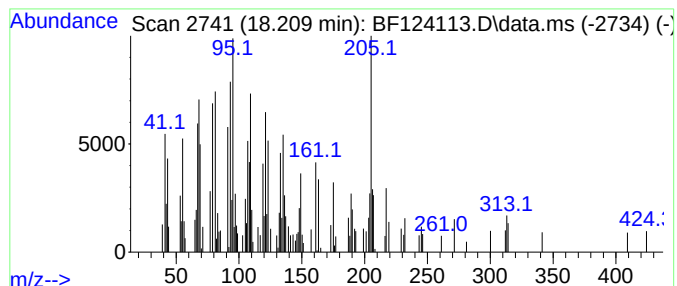
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 unknown18.209 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.209	20.59 ng	344398	Perylene-d12	15.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5.alpha.-Androstan-3.beta.-ol, 4...	304	C21H36O	007673-19-0	27	
2	2-Butenal, 2-methyl-4-(2,6,6-tri...	206	C14H22O	003155-71-3	27	
3	Bis(Methylseleno)methane	204	C3H8Se2	056051-03-7	25	
4	Naphthalene, 1,2,3,5,6,7,8a-oc...	204	C15H24	010219-75-7	25	
5	.alpha.-Bulnesene	204	C15H24	1000374-19-9	20	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
Acq On : 28 May 2021 18:41
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-073

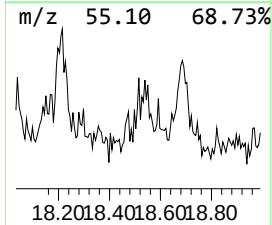
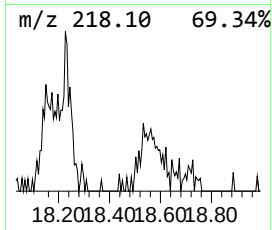
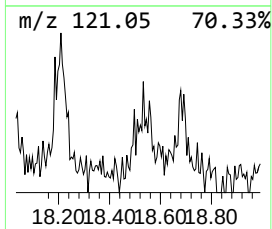
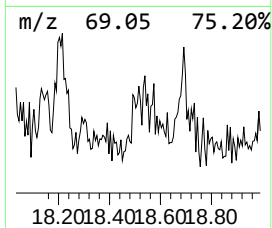
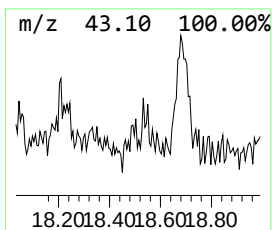
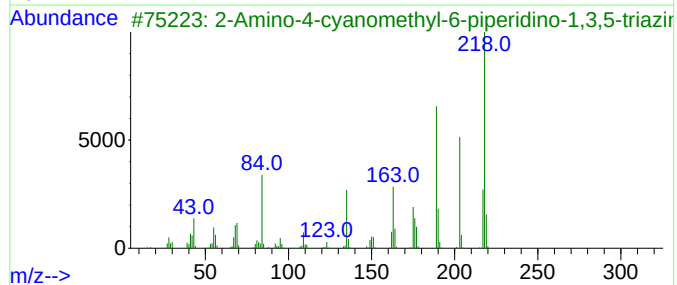
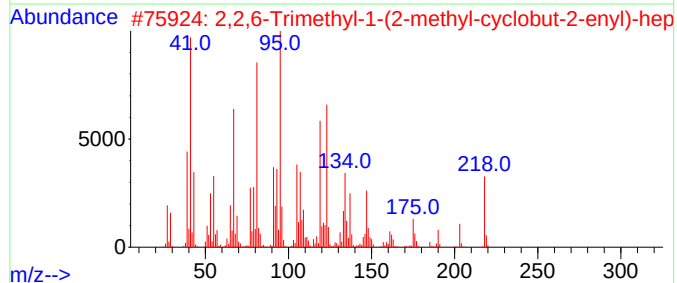
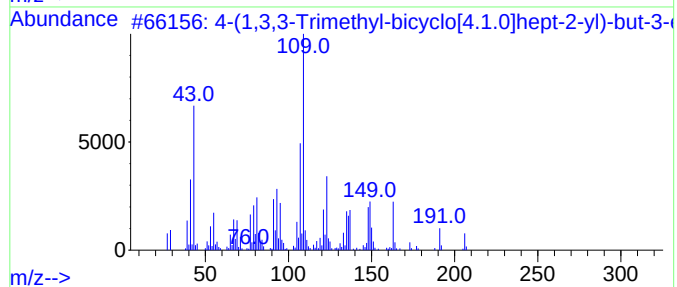
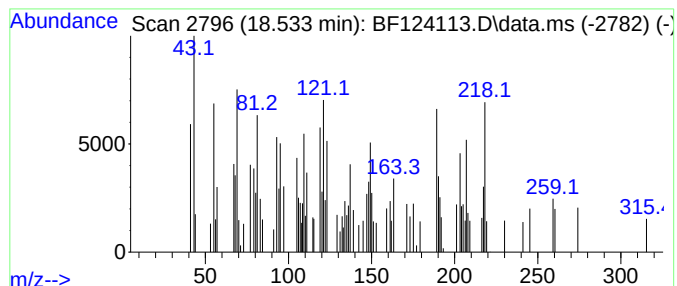
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 unknown18.533 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.533	9.46 ng	158174	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	38		
2	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	35		
3	2-Amino-4-cyanomethyl-6-piperidi...	218	C10H14N6	1000241-05-9	30		
4	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	25		
5	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124113.D
Acq On : 28 May 2021 18:41
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-073

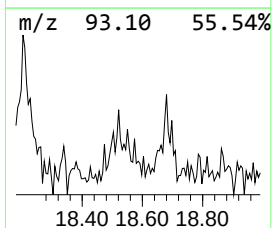
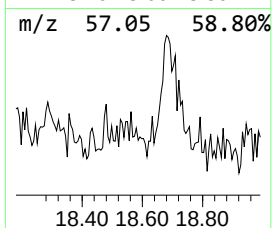
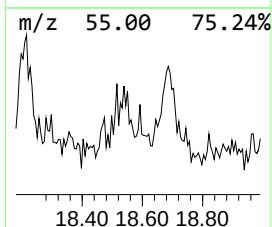
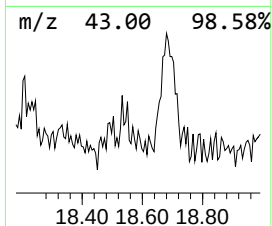
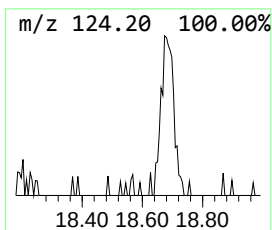
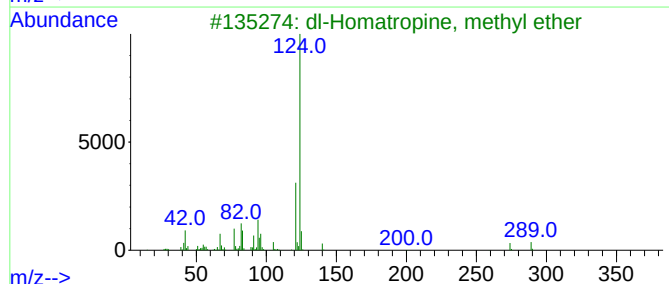
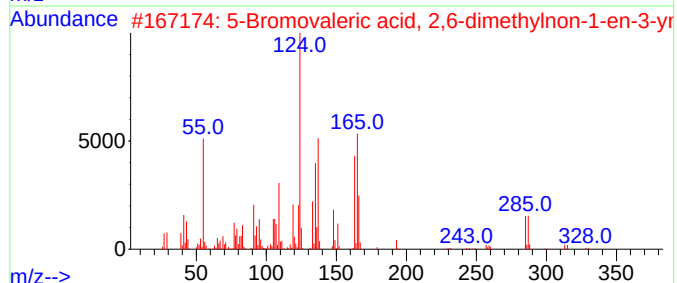
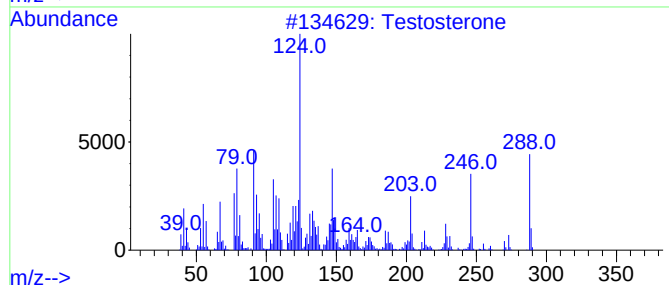
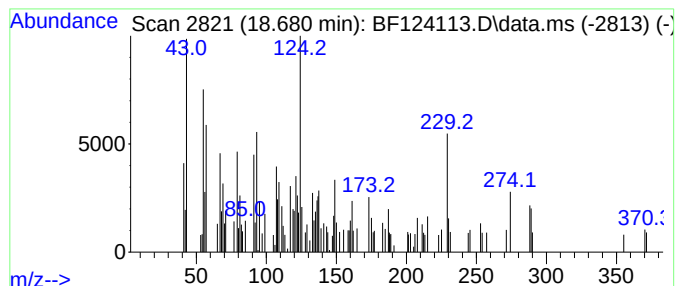
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 unknown18.680 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.680	18.91 ng	316311	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Testosterone	288	C19H28O2	000058-22-0	25
2			5-Bromovaleric acid, 2,6-dimethy...	328	C16H25BrO2	1000292-56-9	25
3			dl-Homatropine, methyl ether	289	C17H23NO3	1000333-83-4	22
4			Testosterone propionate	344	C22H32O3	000057-85-2	22
5			Benzene, 1-(butylthio)-3-methyl-	180	C11H16S	054576-41-9	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
 Data File : BF124113.D
 Acq On : 28 May 2021 18:41
 Operator : JU/CG
 Sample : M2539-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-073

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.140	60.1	ng	590448	1	6.869	196365	20.0
Ethanol, 2-(2-b...	8.057	4.8	ng	51600	2	8.157	215017	20.0
unknown13.645	13.645	20.2	ng	276990	5	14.045	273887	20.0
Octadecane	13.892	3.8	ng	51635	5	14.045	273887	20.0
Diethylene glyc...	13.910	8.9	ng	121307	5	14.045	273887	20.0
Heptacosane	14.204	4.0	ng	54177	5	14.045	273887	20.0
Hexadecane	14.509	5.3	ng	72691	5	14.045	273887	20.0
n-Nonadecanol-1	14.557	6.9	ng	94553	5	14.045	273887	20.0
Sulfurous acid,...	14.821	3.9	ng	65421	6	15.527	334461	20.0
Tetratetracontane	15.168	9.6	ng	160846	6	15.527	334461	20.0
unknown15.762	15.762	4.1	ng	67870	6	15.527	334461	20.0
Hexacosane	16.003	7.2	ng	120086	6	15.527	334461	20.0
unknown16.821	16.821	4.4	ng	74107	6	15.527	334461	20.0
unknown17.333	17.333	6.7	ng	112602	6	15.527	334461	20.0
unknown17.674	17.674	17.0	ng	284909	6	15.527	334461	20.0
unknown17.850	17.850	4.9	ng	81202	6	15.527	334461	20.0
unknown18.027	18.027	3.8	ng	63481	6	15.527	334461	20.0
unknown18.209	18.209	20.6	ng	344398	6	15.527	334461	20.0
unknown18.533	18.533	9.5	ng	158174	6	15.527	334461	20.0
unknown18.680	18.680	18.9	ng	316311	6	15.527	334461	20.0