

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042919\
 Data File : BF114027.D
 Acq On : 29 Apr 2019 17:18
 Operator : JU/SJ
 Sample : K2553-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR200034

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF042219.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	15	19	24	rVB	53575	74164	2.48%	0.270%
2	5.516	578	583	587	rBV	2188254	2127210	71.04%	7.750%
3	6.522	748	754	757	rBV	2341588	2250871	75.17%	8.200%
4	6.663	773	778	781	rBV	2717121	2391453	79.87%	8.712%
5	6.892	813	817	821	rBV	906770	708061	23.65%	2.580%
6	7.051	840	844	847	rBV	2319226	1920515	64.14%	6.997%
7	7.451	907	912	915	rBV	1529944	1426397	47.64%	5.197%
8	8.175	1031	1035	1048	rBV	931578	898086	29.99%	3.272%
9	9.245	1213	1217	1220	rBV	3499331	2994347	100.00%	10.909%
10	9.633	1280	1283	1292	rVB	376019	328331	10.97%	1.196%
11	9.922	1328	1332	1343	rVB	1222843	1098708	36.69%	4.003%
12	10.710	1461	1466	1480	rBV	2083370	1895918	63.32%	6.907%
13	11.410	1580	1585	1587	rBV	1160373	1138849	38.03%	4.149%
14	11.427	1587	1588	1592	rVB	141233	101636	3.39%	0.370%
15	11.927	1670	1673	1682	rVB2	252798	266887	8.91%	0.972%
16	12.616	1787	1790	1796	rBV	242885	237867	7.94%	0.867%
17	12.716	1803	1807	1821	rBV2	142537	182086	6.08%	0.663%
18	12.845	1824	1829	1835	rVB	205501	215161	7.19%	0.784%
19	12.992	1849	1854	1857	rBV	3207876	2950462	98.53%	10.749%
20	13.680	1968	1971	1976	rVB2	34056	35470	1.18%	0.129%
21	13.892	2004	2007	2008	rBV2	38351	39774	1.33%	0.145%
22	13.921	2008	2012	2022	rVB7	59104	155767	5.20%	0.567%
23	14.045	2028	2033	2036	rBV	1011189	998829	33.36%	3.639%
24	14.068	2036	2037	2043	rVB	113750	84888	2.83%	0.309%
25	14.527	2110	2115	2118	rBV2	72352	81548	2.72%	0.297%
26	14.568	2118	2122	2129	rVV9	29933	73017	2.44%	0.266%
27	14.686	2139	2142	2146	rBV2	31850	41392	1.38%	0.151%
28	14.839	2165	2168	2172	rVB	94611	94438	3.15%	0.344%
29	14.986	2190	2193	2196	rVB2	51361	45363	1.51%	0.165%
30	15.104	2208	2213	2221	rVB	97368	194852	6.51%	0.710%
31	15.180	2222	2226	2230	rBV	134950	152530	5.09%	0.556%
32	15.257	2234	2239	2248	rBV9	36615	99432	3.32%	0.362%
33	15.404	2261	2264	2270	rVB	61414	84999	2.84%	0.310%
34	15.468	2271	2275	2281	rVV	69699	91846	3.07%	0.335%

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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

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35	15.539	2281	2287	2290	rVV	696015	955214	31.90%	3.480%
36	15.568	2290	2292	2298	rVB	143178	167806	5.60%	0.611%
37	15.768	2323	2326	2331	rVB6	30495	41342	1.38%	0.151%
38	16.015	2362	2368	2374	rBV	126410	197565	6.60%	0.720%
39	16.527	2449	2455	2459	rBV3	70781	119875	4.00%	0.437%
40	16.815	2501	2504	2510	rBV7	20632	35759	1.19%	0.130%
41	17.009	2533	2537	2544	rVB2	36104	65249	2.18%	0.238%
42	17.127	2553	2557	2564	rVB3	37450	78224	2.61%	0.285%
43	17.251	2574	2578	2584	rBV6	23693	49068	1.64%	0.179%
44	17.456	2609	2613	2624	rVB	34880	75727	2.53%	0.276%
45	18.168	2727	2734	2747	rVB7	31313	108381	3.62%	0.395%
46	18.674	2815	2820	2829	rVB9	28169	73574	2.46%	0.268%

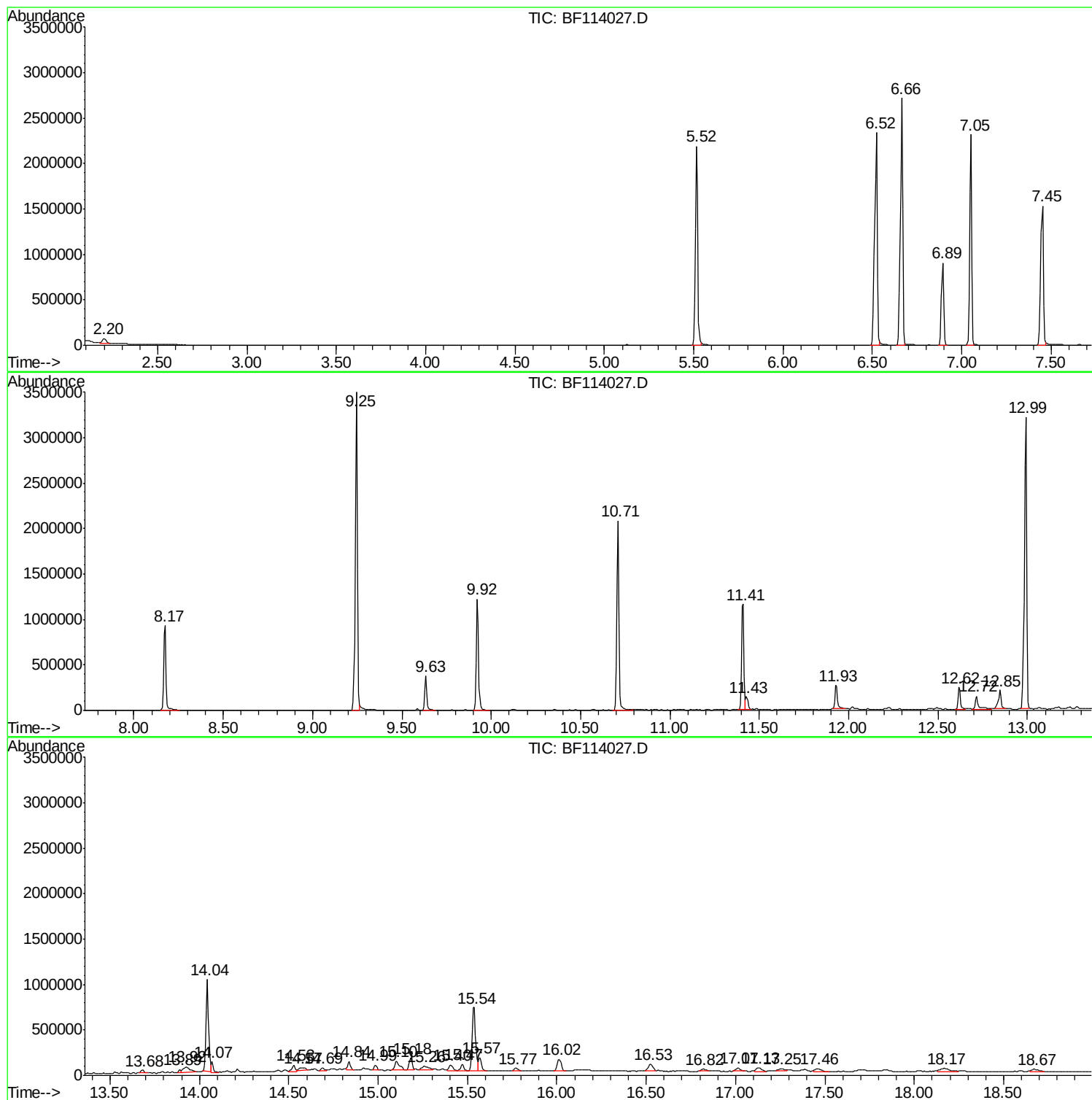
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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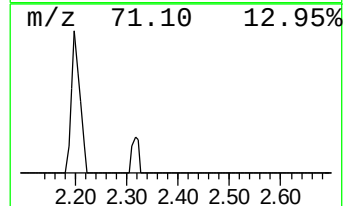
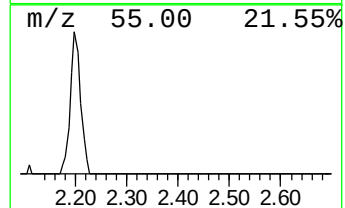
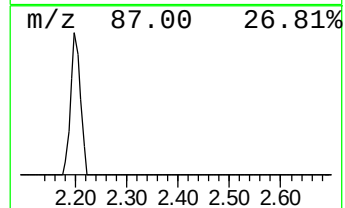
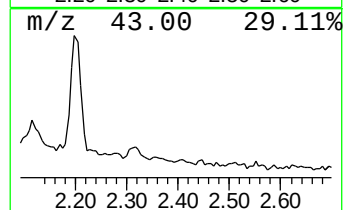
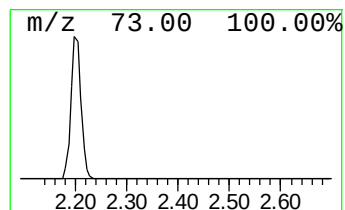
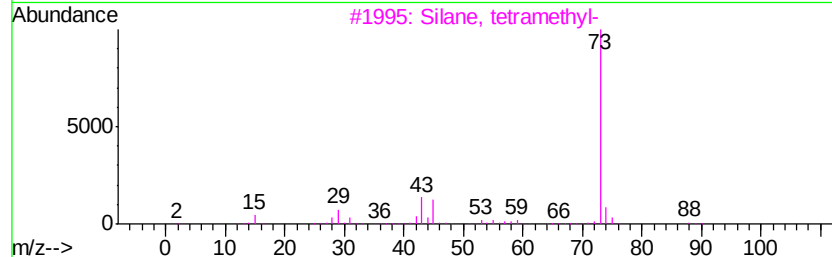
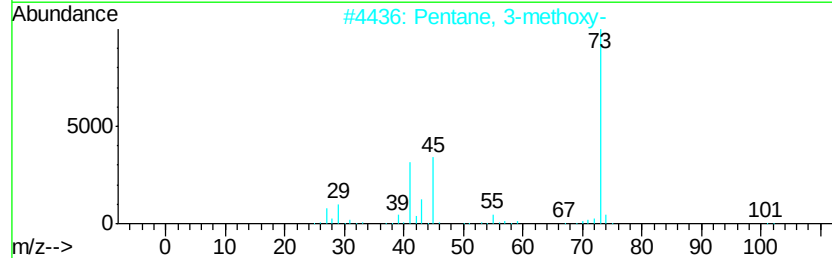
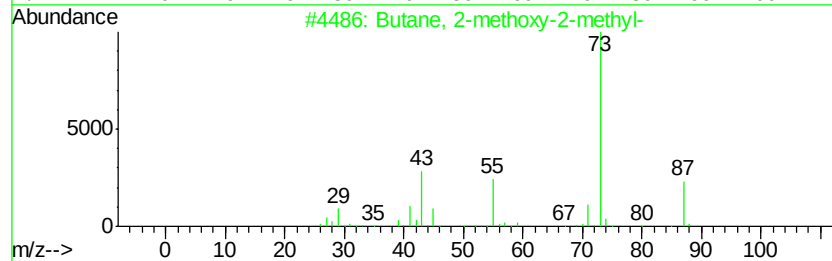
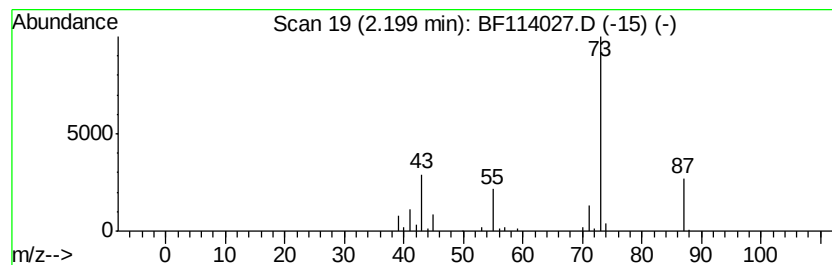
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	2.09 ng	74164	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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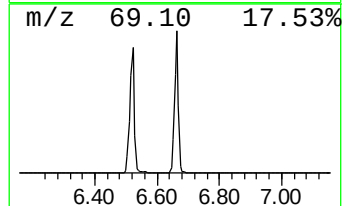
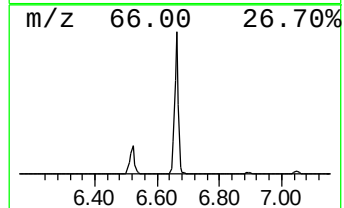
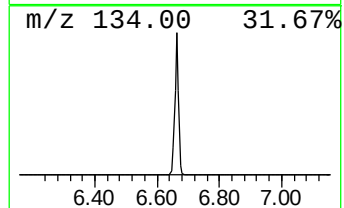
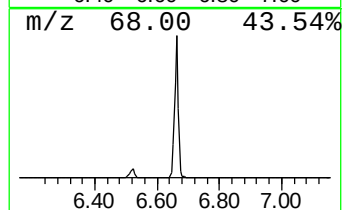
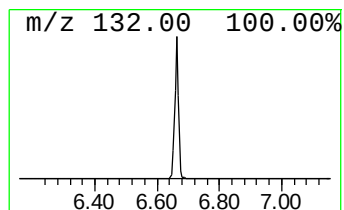
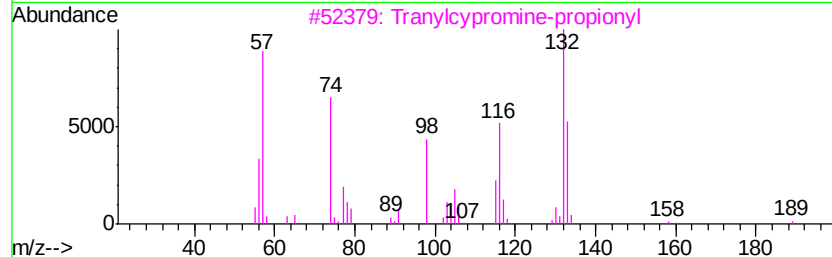
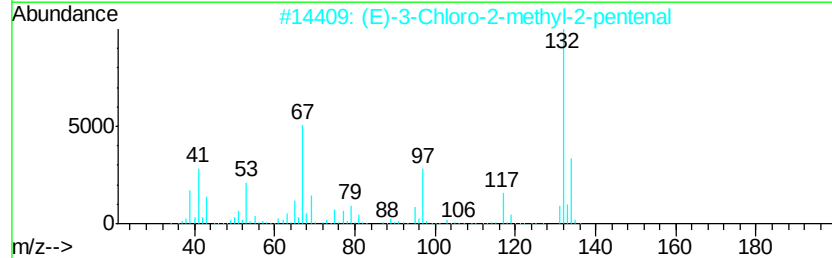
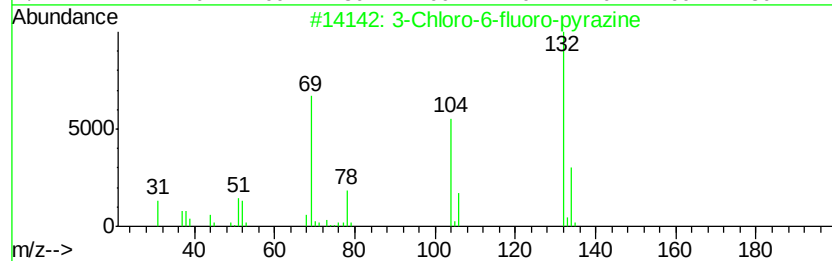
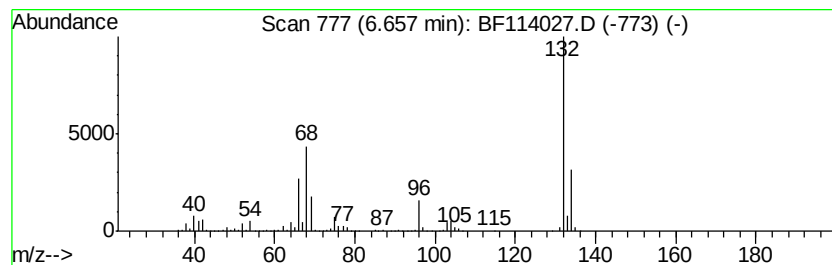
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	67.55 ng	2391450	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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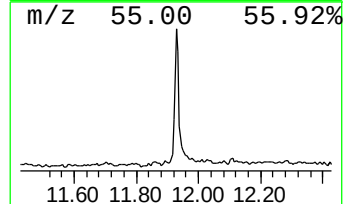
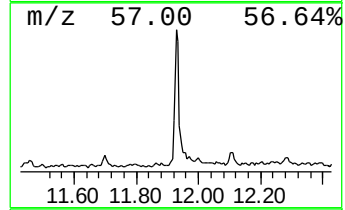
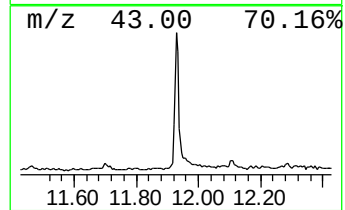
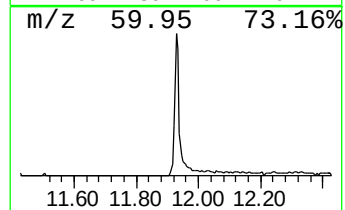
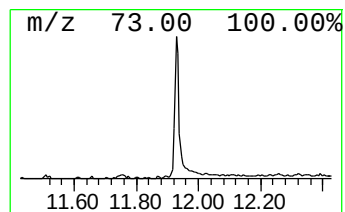
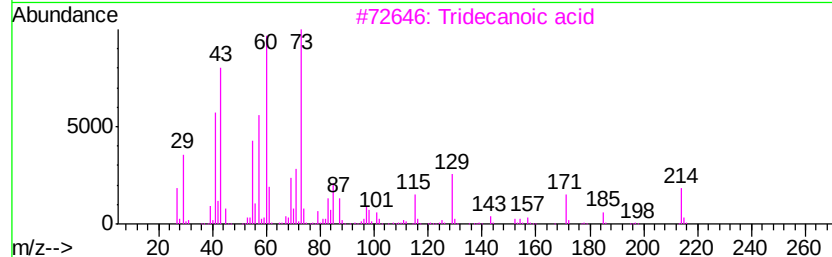
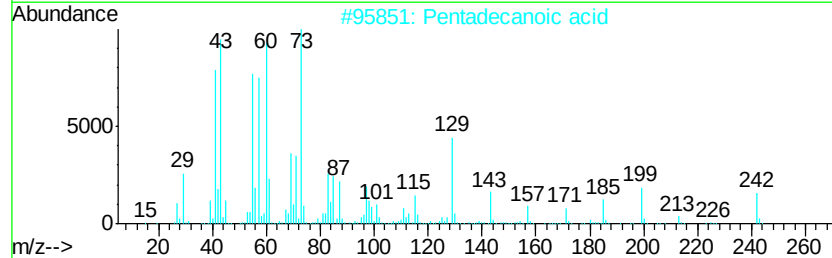
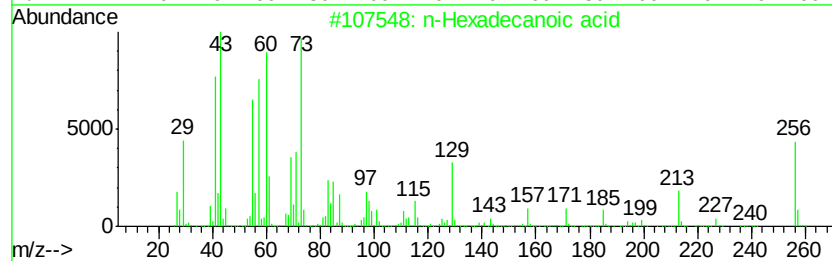
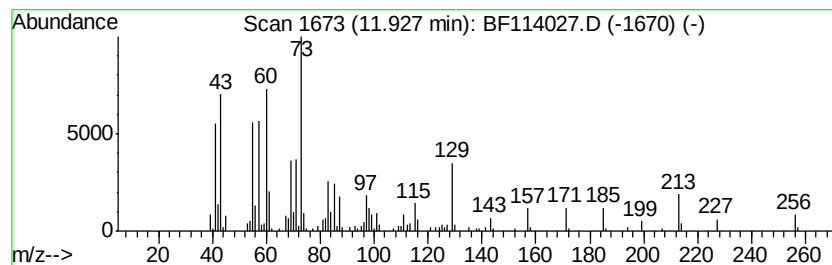
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	4.69 ng	266887	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3		Tridecanoic acid	214	C13H26O2	000638-53-9	74
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



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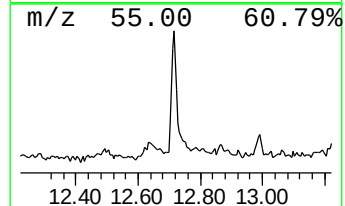
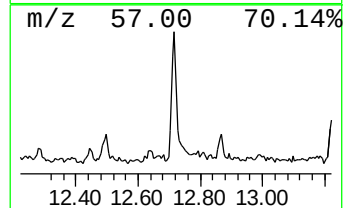
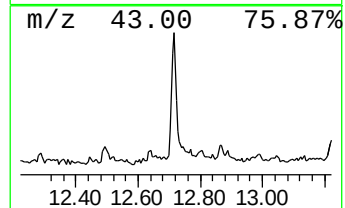
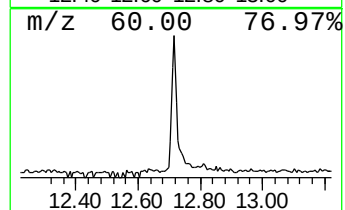
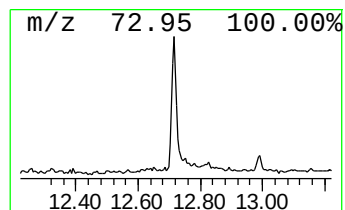
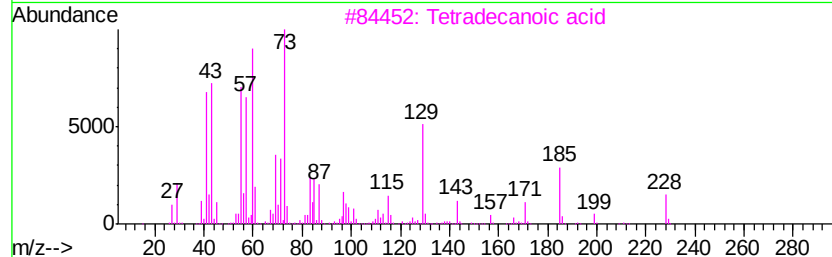
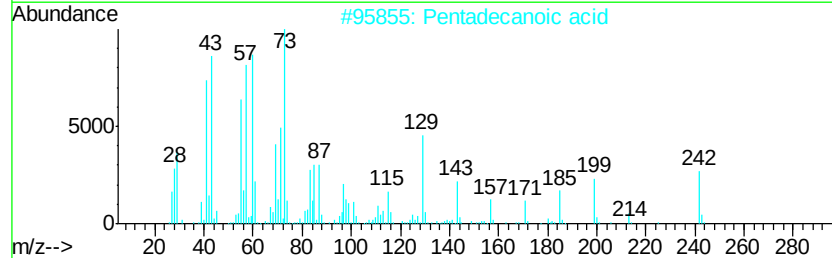
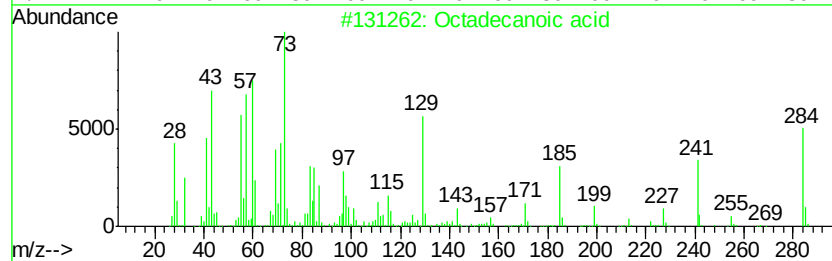
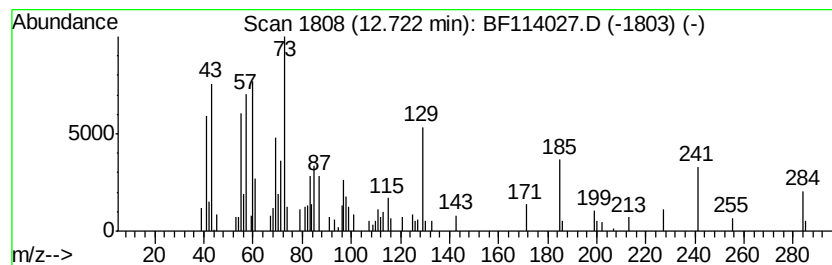
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	3.20 ng	182086	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		n-Decanoic acid	172	C10H20O2	000334-48-5	64
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52



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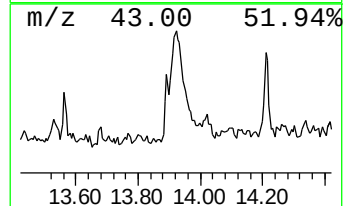
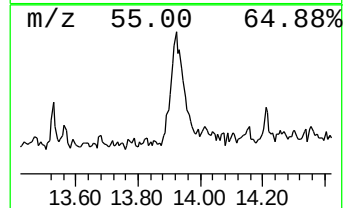
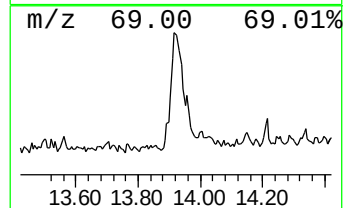
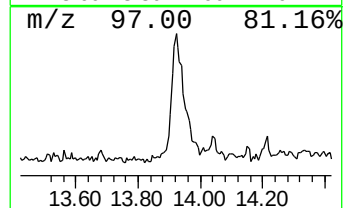
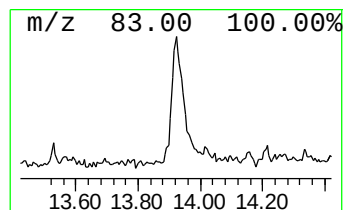
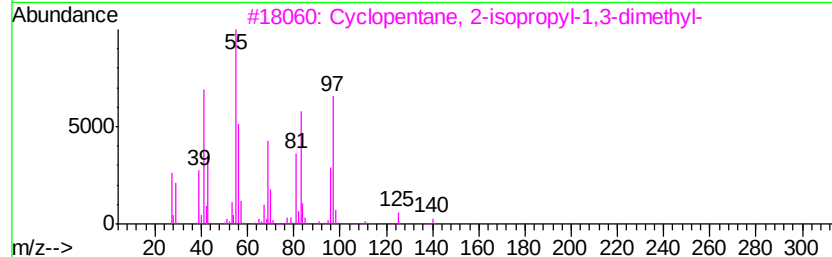
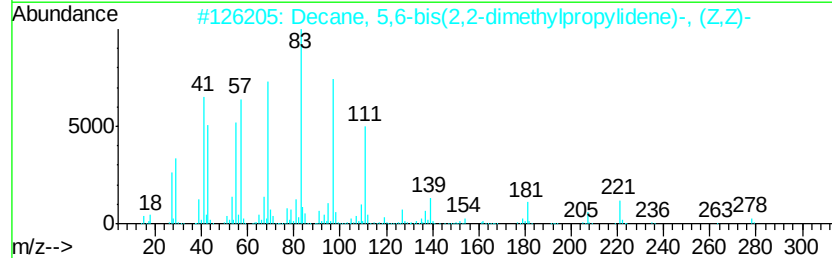
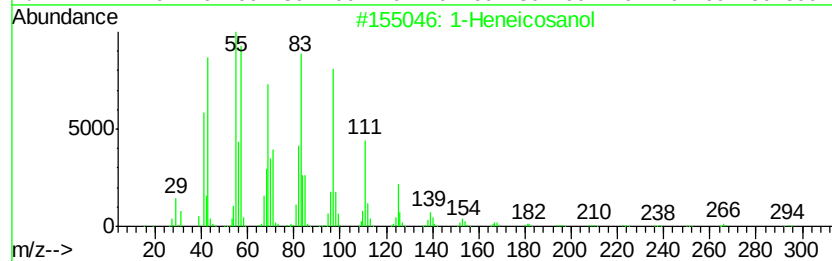
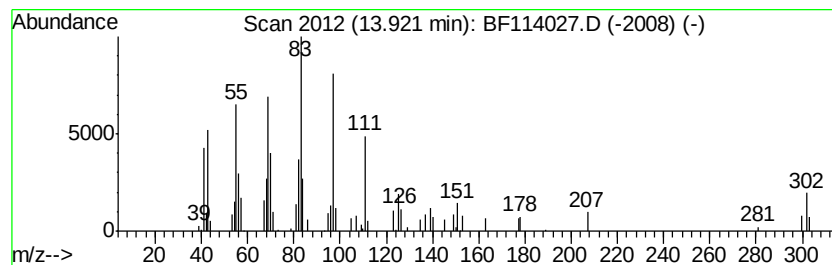
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	3.12 ng	155767	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	83
2		Decane, 5,6-bis(2,2-dimethylprop...	278	C20H38	073002-85-4	52
3		Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	49
4		Cyclohexanone, 3-ethyl-	126	C8H14O	022461-89-8	38
5		Benzene, 1-fluoro-4-methoxy-	126	C7H7FO	000459-60-9	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042919\
Data File : BF114027.D
Acq On : 29 Apr 2019 17:18
Operator : JU/SJ
Sample : K2553-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200034

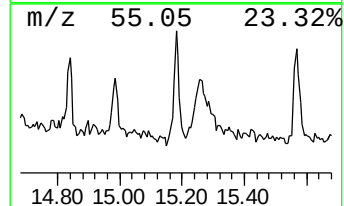
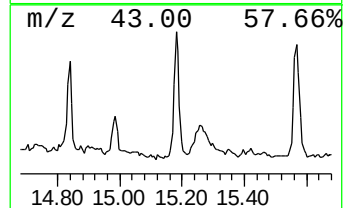
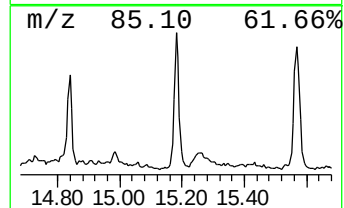
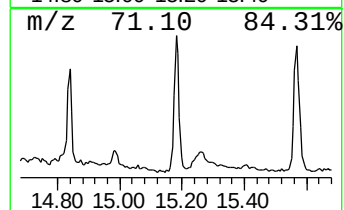
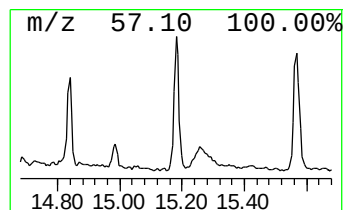
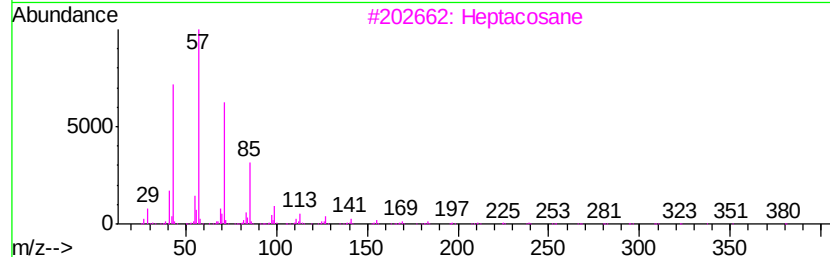
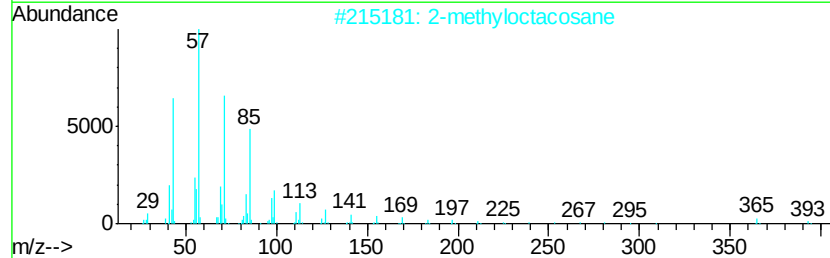
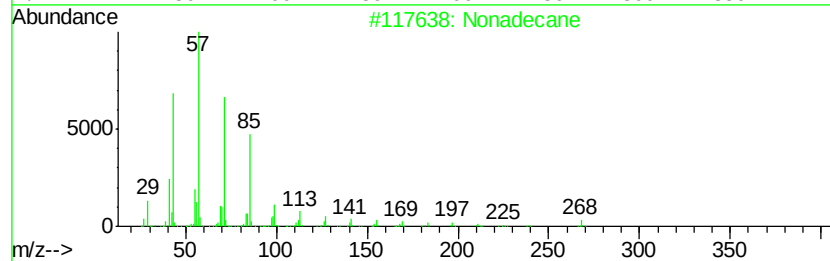
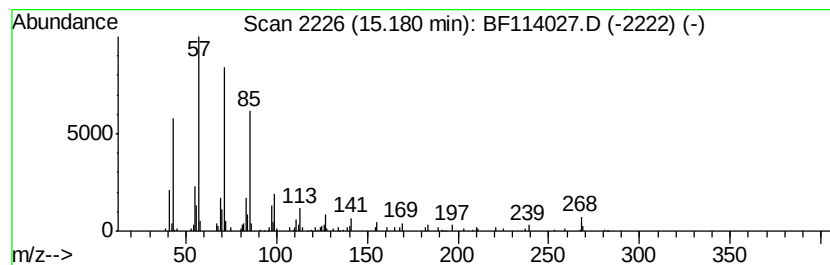
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	3.19 ng	152530	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042919\
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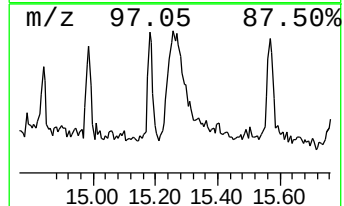
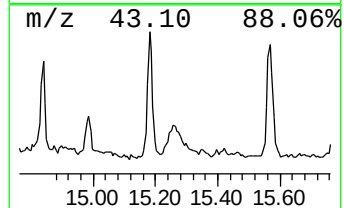
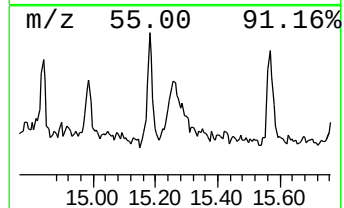
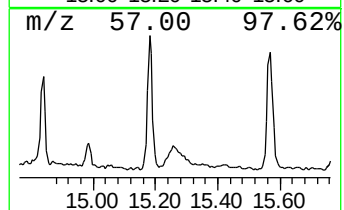
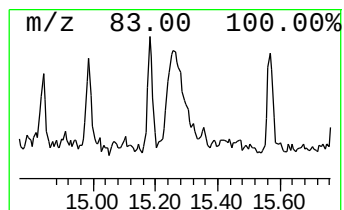
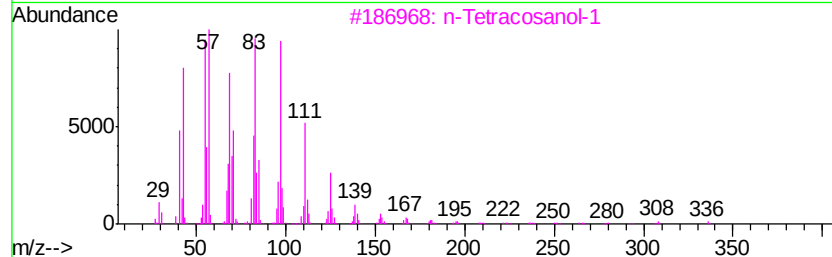
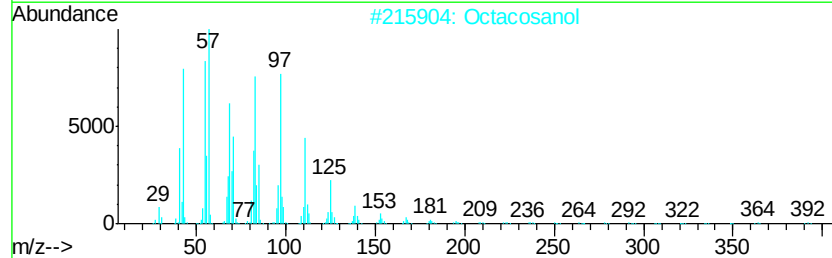
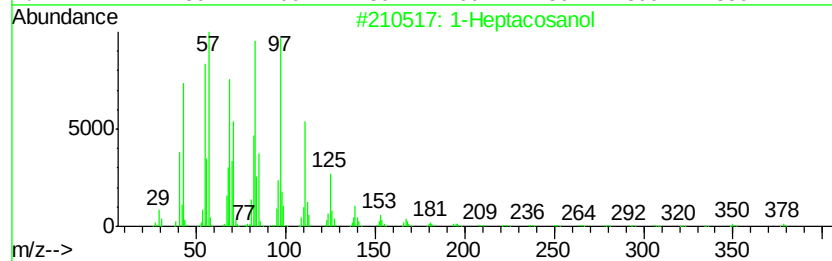
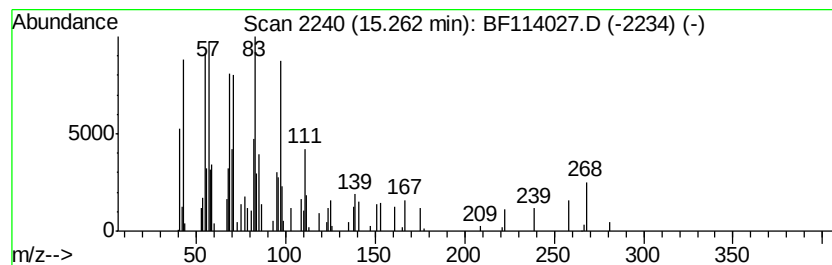
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heptacosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.26	2.08 ng	99432	Perylene-d12		15.54
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	81
2	Octacosanol	410	C28H58O	000557-61-9	76
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	76
4	1-Heneicosanol	312	C21H44O	015594-90-8	76
5	Behenic alcohol	326	C22H46O	000661-19-8	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042919\
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Sample : K2553-01
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Instrument :
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ClientSampleId :
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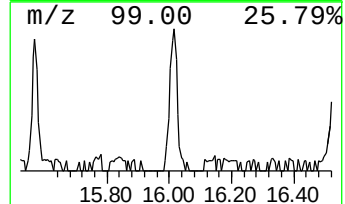
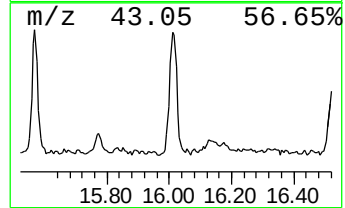
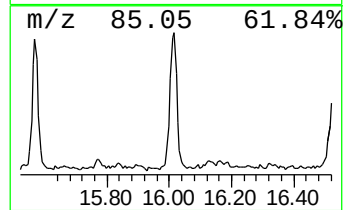
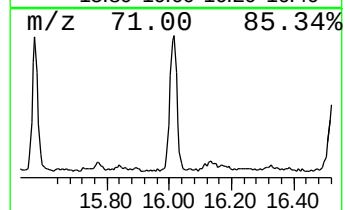
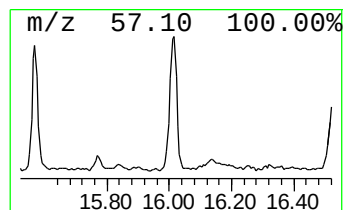
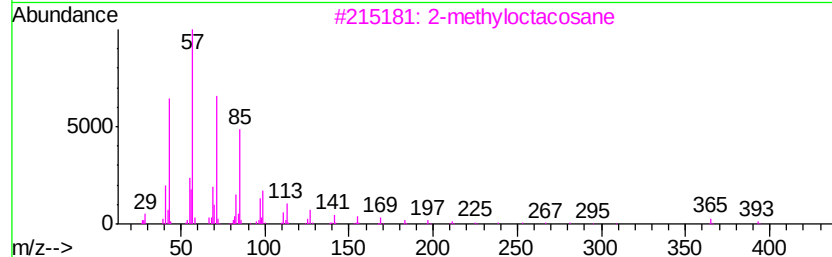
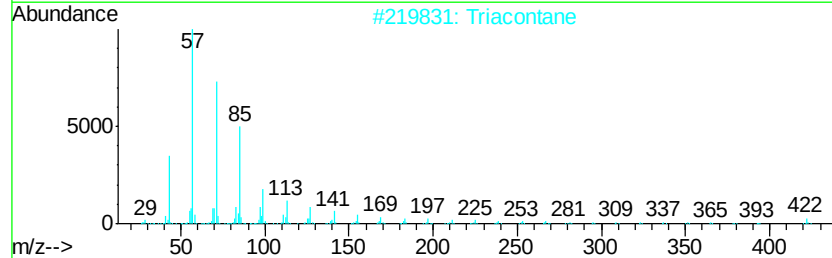
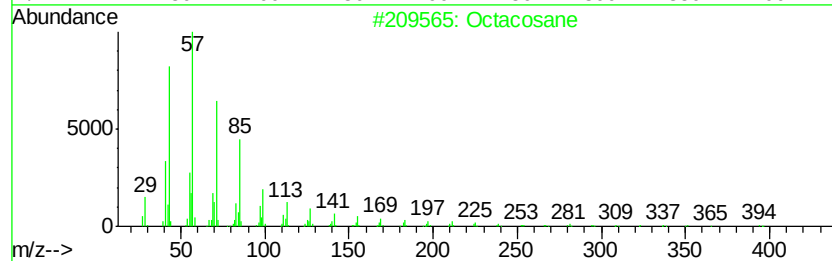
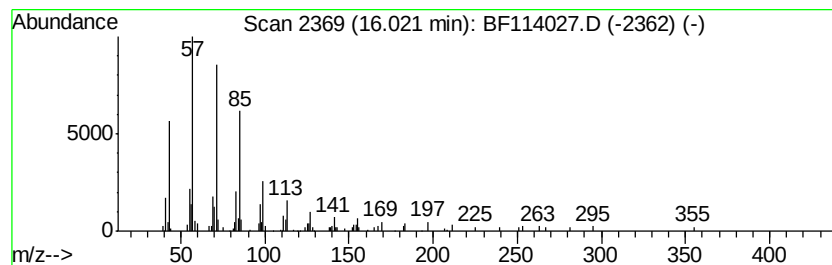
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	4.14 ng	197565	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Triacontane	422	C30H62	000638-68-6	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042919\
Data File : BF114027.D
Acq On : 29 Apr 2019 17:18
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Sample : K2553-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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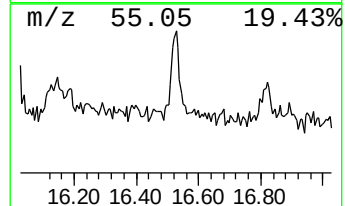
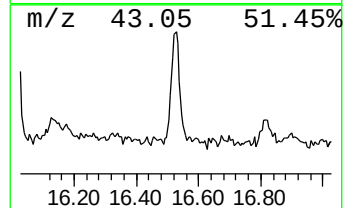
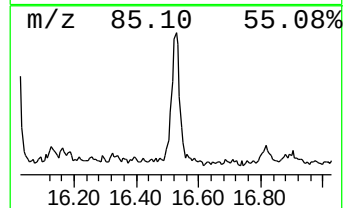
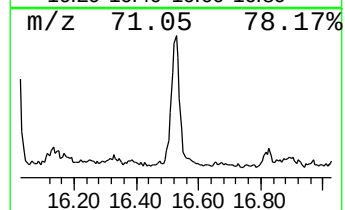
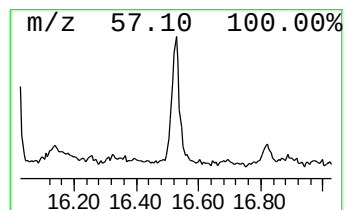
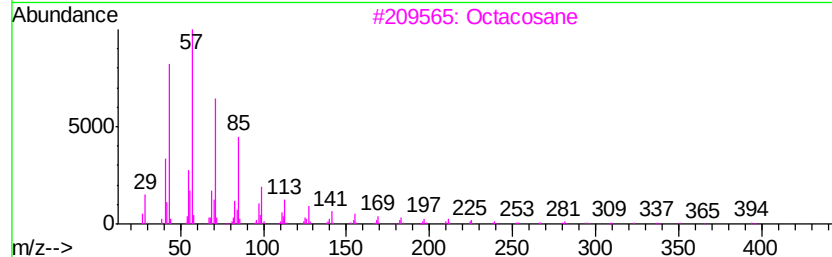
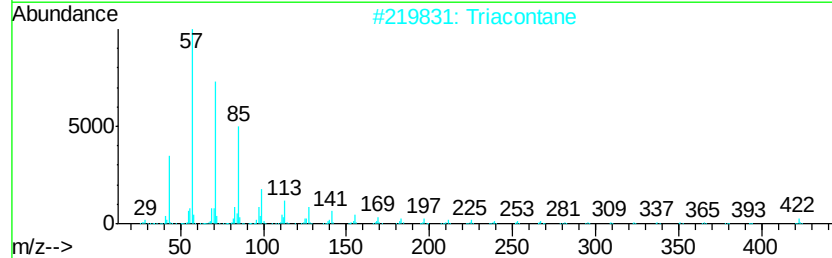
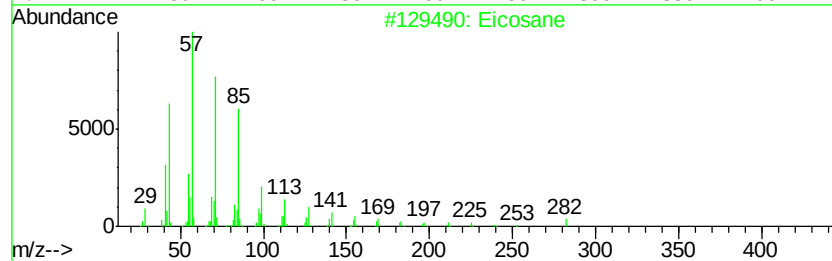
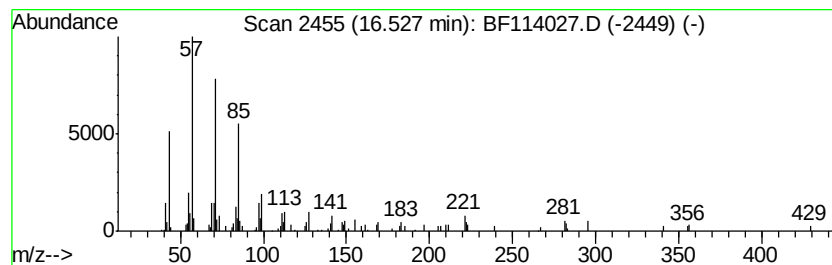
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.51 ng	119875	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	98
2		Triacontane	422	C30H62	000638-68-6	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	87
5		Docosane, 11-decyl-	451	C32H66	055401-55-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042919\
Data File : BF114027.D
Acq On : 29 Apr 2019 17:18
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Sample : K2553-01
Misc :
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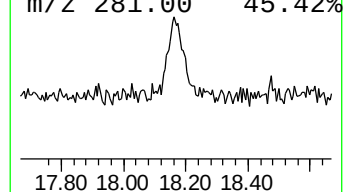
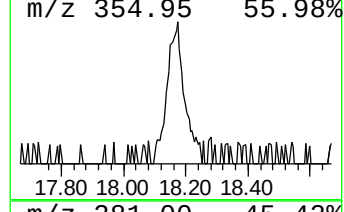
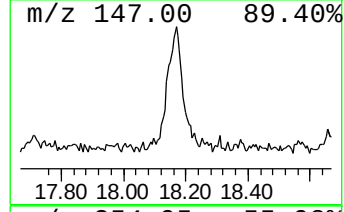
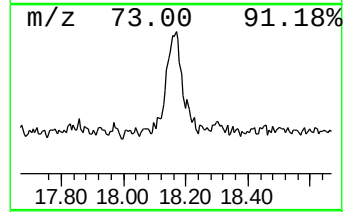
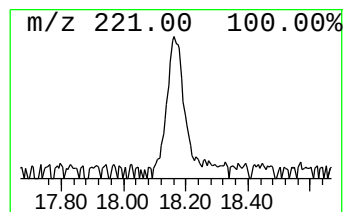
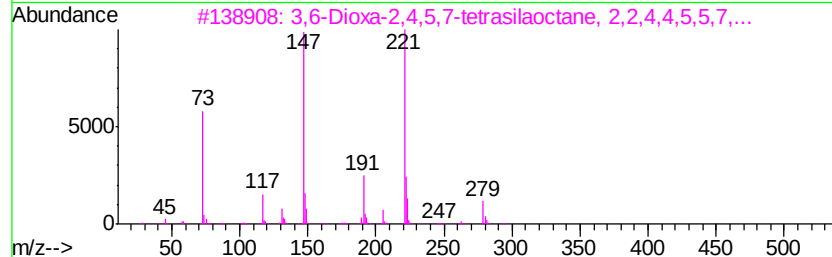
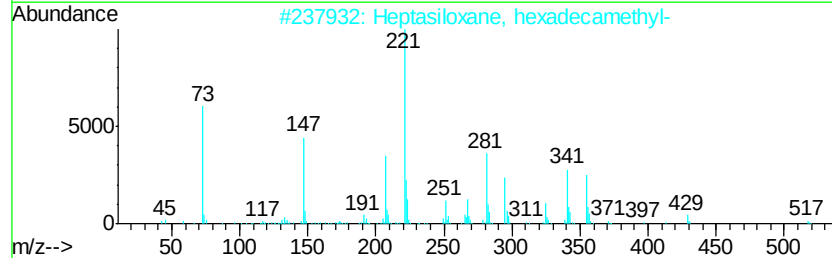
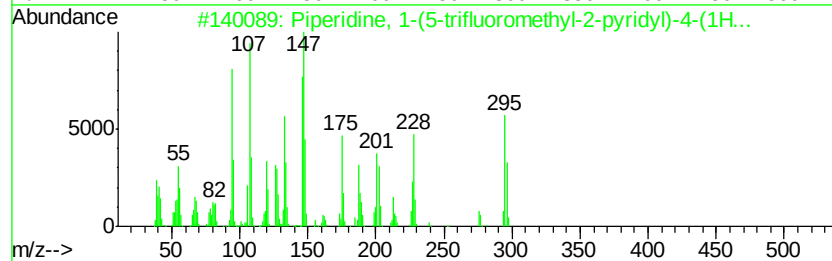
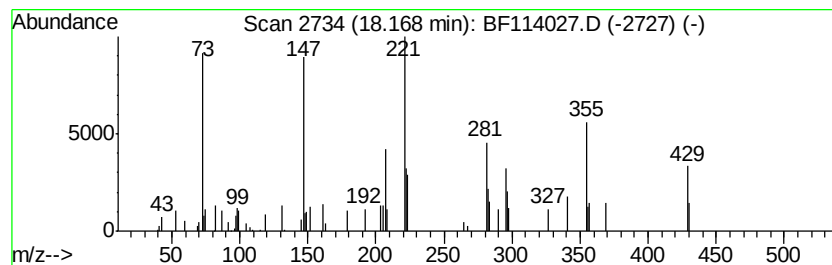
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Piperidine, 1-(5-trifluoromethyl-2-pyridyl)-4-(1H... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.17	2.27 ng	108381	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Piperidine, 1-(5-trifluoromethyl-2-pyridyl)-4-(1H...	295	C15H16F3N3	1000268-74-7	74
2		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	42
3		3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octa-	294	C10H30O2Si4	004342-25-0	32
4		Thioxanthene, 9-(tetrahydrothiophen-2-yl)-	296	C18H16S2	116196-88-4	25
5		Trisiloxane, 1,1,1,5,5,5-hexamethyl-3-(trimethylsilyl)-	384	C12H36O4Si5	003555-47-3	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042919\
Data File : BF114027.D
Acq On : 29 Apr 2019 17:18
Operator : JU/SJ
Sample : K2553-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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
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unknown6.66	6.66	67.5 ng		2391450	1	6.89	708061	20.0
n-Hexadecanoic acid	11.93	4.7 ng		266887	4	11.41	1138850	20.0
Octadecanoic acid	12.72	3.2 ng		182086	4	11.41	1138850	20.0
1-Heneicosanol	13.92	3.1 ng		155767	5	14.04	998829	20.0
Nonadecane	15.18	3.2 ng		152530	6	15.54	955214	20.0
1-Heptacosanol	15.26	2.1 ng		99432	6	15.54	955214	20.0
Octacosane	16.02	4.1 ng		197565	6	15.54	955214	20.0
Eicosane	16.53	2.5 ng		119875	6	15.54	955214	20.0
Piperidine, 1-(5-...	18.17	2.3 ng		108381	6	15.54	955214	20.0