

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
 Data File : BF130856.D
 Acq On : 29 Oct 2022 14:43
 Operator : CG\JU
 Sample : N5332-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-4-WC

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130856.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.275	26	32	38	rVB	550777	728745	32.47%	3.963%
2	2.393	48	52	61	rVB	37272	49689	2.21%	0.270%
3	5.175	517	525	533	rBV	372425	446074	19.88%	2.426%
4	5.557	585	590	593	rBV	2120004	2086855	92.99%	11.349%
5	6.557	754	760	763	rBV	2112859	2196202	97.86%	11.944%
6	6.940	822	825	829	rBV	661767	547928	24.42%	2.980%
7	7.504	916	921	924	rBV	1493068	1340463	59.73%	7.290%
8	8.228	1040	1044	1047	rBV	854376	685248	30.53%	3.727%
9	9.304	1222	1227	1230	rBV	2753396	2244186	100.00%	12.205%
10	9.986	1339	1343	1346	rBV	901870	703285	31.34%	3.825%
11	10.775	1473	1477	1480	rBV	1444718	1180212	52.59%	6.419%
12	10.880	1492	1495	1501	rBV2	37297	40827	1.82%	0.222%
13	11.475	1593	1596	1599	rBV	696897	616914	27.49%	3.355%
14	11.498	1599	1600	1604	rVV	144445	91233	4.07%	0.496%
15	11.551	1604	1609	1613	rVB2	26797	32396	1.44%	0.176%
16	11.863	1659	1662	1665	rBV	64002	49671	2.21%	0.270%
17	11.992	1679	1684	1690	rBV2	115144	162650	7.25%	0.885%
18	12.092	1697	1701	1703	rBV2	34089	37409	1.67%	0.203%
19	12.574	1778	1783	1787	rBV5	45966	58802	2.62%	0.320%
20	12.692	1799	1803	1808	rVB	311724	258127	11.50%	1.404%
21	12.780	1815	1818	1822	rBV3	39280	38167	1.70%	0.208%
22	12.921	1836	1842	1846	rBV	250369	265232	11.82%	1.442%
23	12.957	1846	1848	1855	rVB3	44896	48264	2.15%	0.262%
24	13.069	1863	1867	1870	rVB	1605517	1485242	66.18%	8.078%
25	13.145	1873	1880	1882	rBV4	21053	40600	1.81%	0.221%
26	13.292	1902	1905	1907	rBV	43504	35825	1.60%	0.195%
27	13.357	1912	1916	1918	rBV2	26630	29886	1.33%	0.163%
28	13.527	1940	1945	1946	rBV4	25930	28123	1.25%	0.153%
29	13.633	1959	1963	1966	rBV2	53288	60889	2.71%	0.331%
30	13.757	1981	1984	1987	rVB	28999	30799	1.37%	0.168%
31	13.874	1999	2004	2006	rBV2	20805	29197	1.30%	0.159%
32	13.963	2016	2019	2022	rBV	89500	78009	3.48%	0.424%
33	14.021	2022	2029	2040	rVV5	65259	228708	10.19%	1.244%
34	14.121	2040	2046	2049	rVV2	599829	654842	29.18%	3.561%
35	14.145	2049	2050	2056	rVB	126751	111301	4.96%	0.605%
36	14.221	2057	2063	2068	rBV2	164353	214154	9.54%	1.165%

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MH-4-WC

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.280	2070	2073	2077	rVB	59520	56914	2.54%	0.310%
38	14.586	2122	2125	2131	rBV3	62513	71115	3.17%	0.387%
39	14.892	2174	2177	2179	rBV	86978	104835	4.67%	0.570%
40	14.992	2191	2194	2197	rBV3	29259	29267	1.30%	0.159%
41	15.186	2223	2227	2230	rBV	120162	175474	7.82%	0.954%
42	15.268	2237	2241	2244	rBV2	60751	68824	3.07%	0.374%
43	15.504	2277	2281	2287	rVB	67026	87983	3.92%	0.479%
44	15.568	2288	2292	2299	rVV	84215	106991	4.77%	0.582%
45	15.639	2299	2304	2307	rVV	334408	409058	18.23%	2.225%
46	15.674	2307	2310	2315	rVB3	66995	92796	4.13%	0.505%
47	16.139	2385	2389	2394	rBV	46066	65726	2.93%	0.357%
48	16.680	2476	2481	2486	rBV3	32361	66719	2.97%	0.363%
49	17.168	2560	2564	2570	rBV	35502	69341	3.09%	0.377%
50	17.639	2640	2644	2650	rVB	26165	46032	2.05%	0.250%

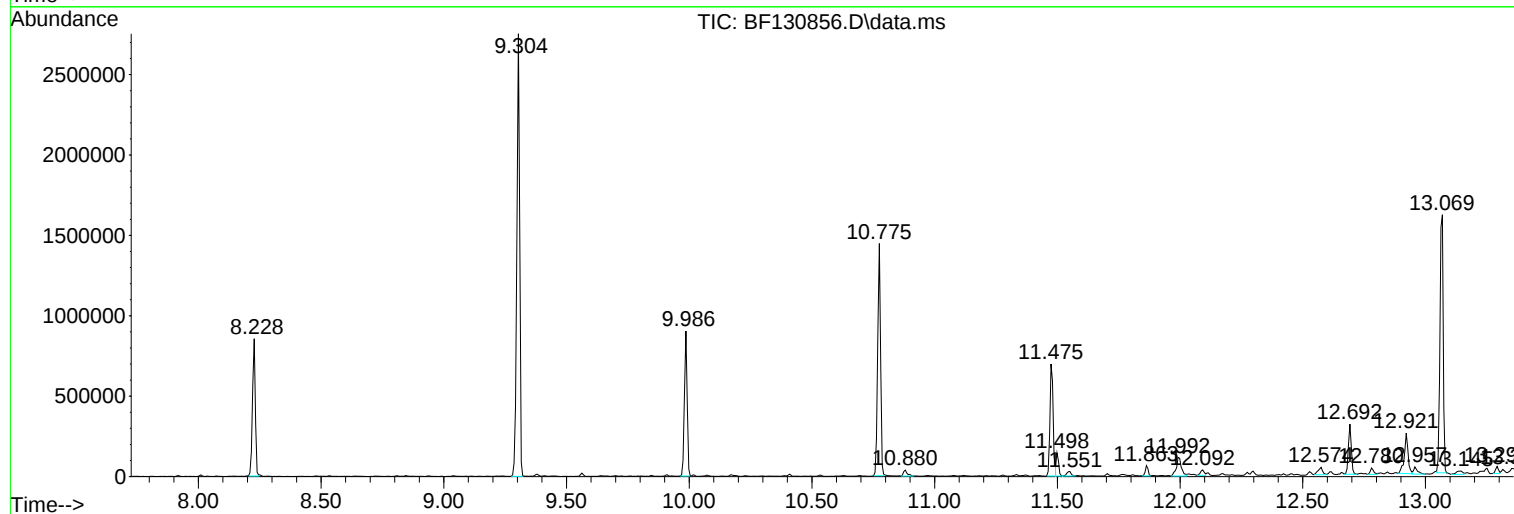
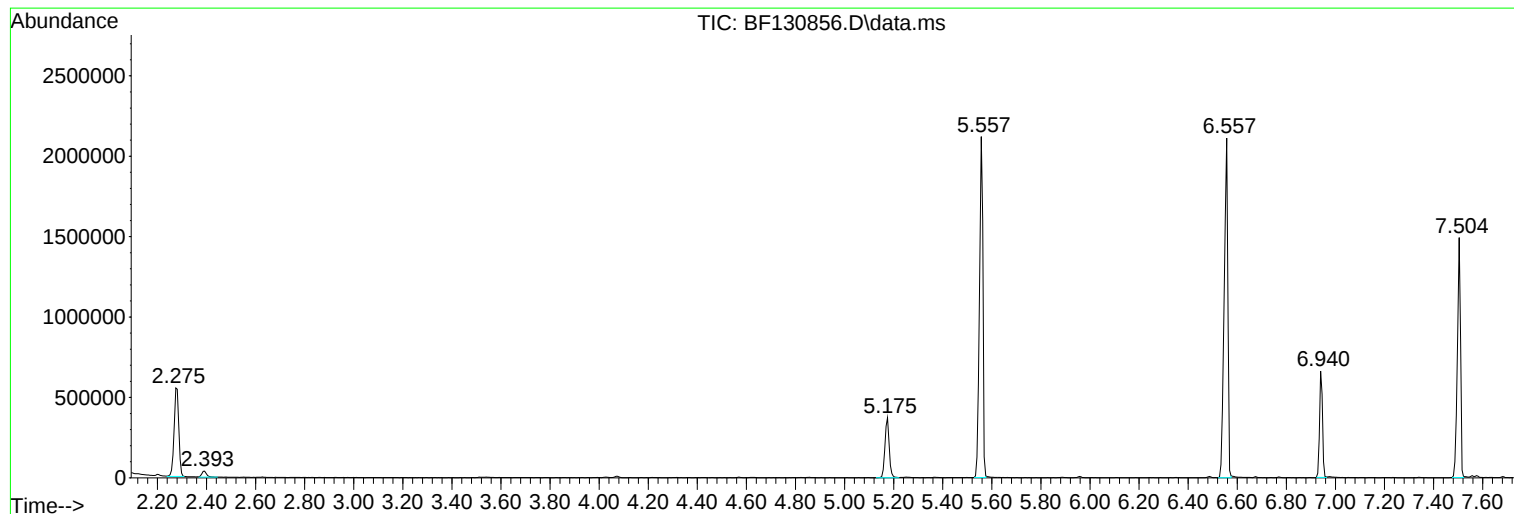
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Operator : CG\JU
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Instrument :
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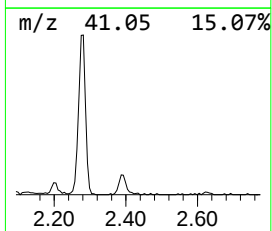
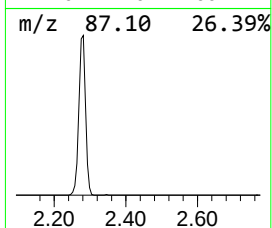
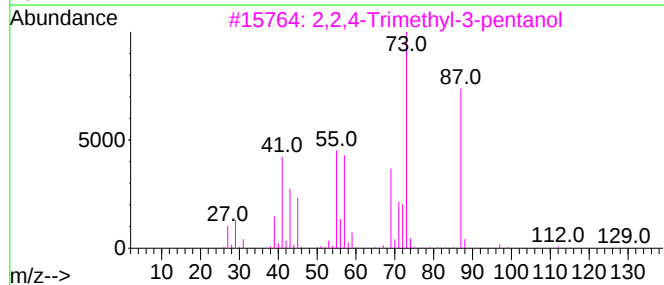
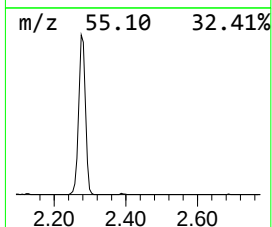
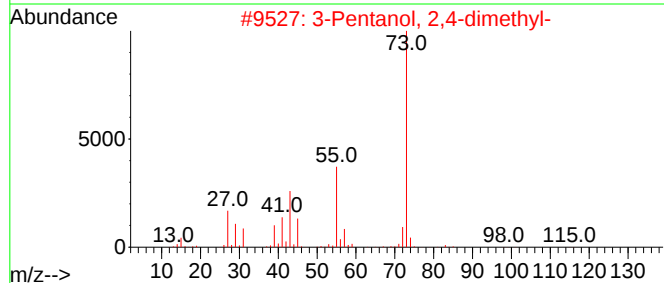
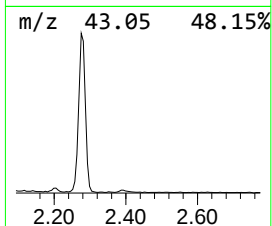
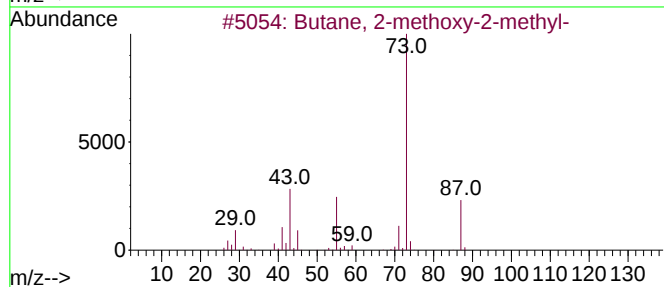
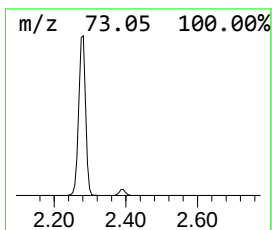
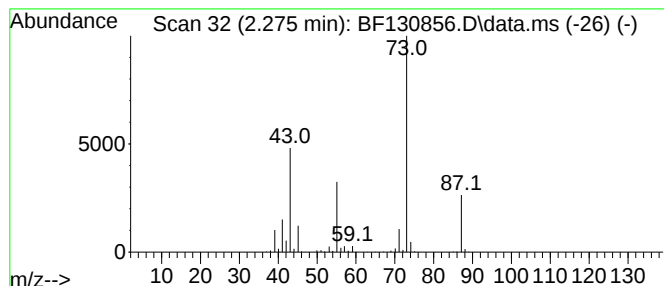
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
2.275	26.60 ng	728745	1,4-Dichlorobenzene-d4	6.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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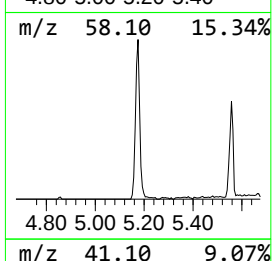
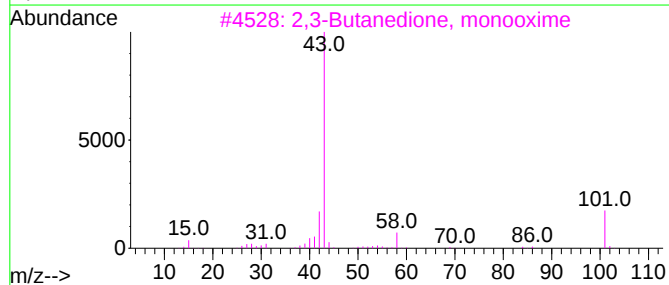
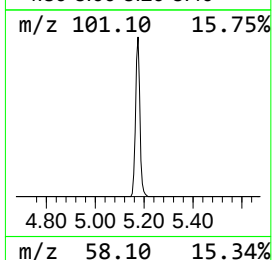
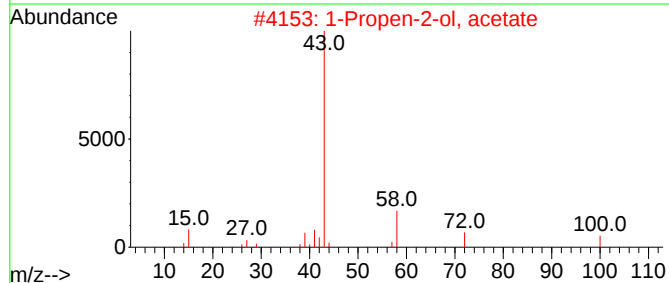
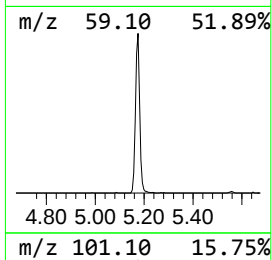
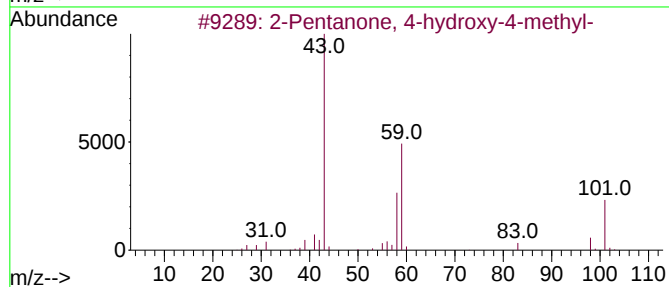
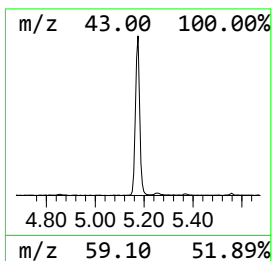
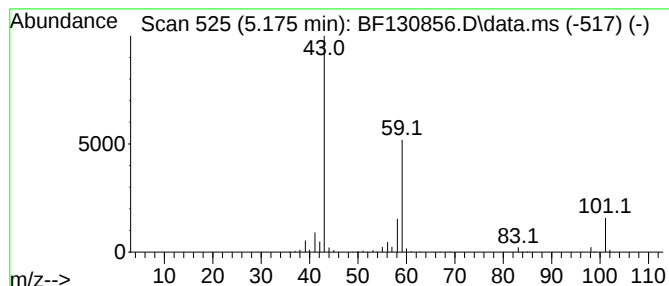
Instrument :
BNA_F
ClientSampleId :
MH-4-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.175	16.28 ng	446074	1,4-Dichlorobenzene-d4	6.940	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9



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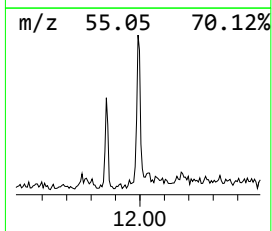
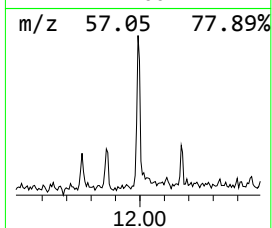
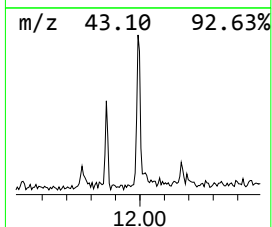
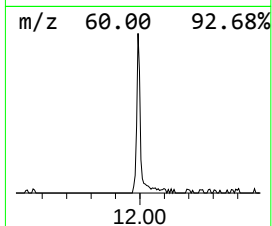
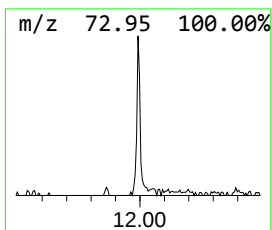
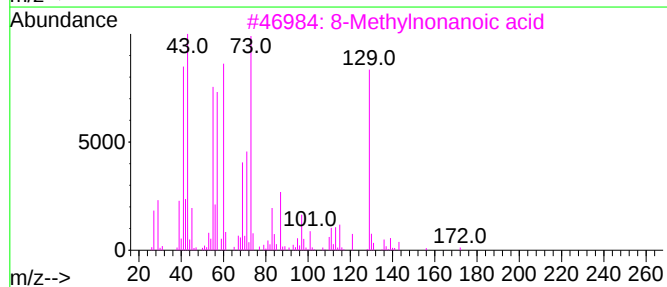
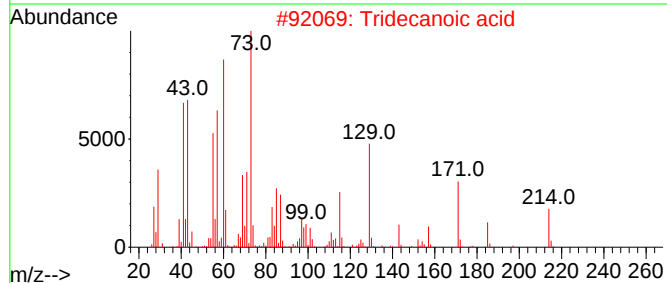
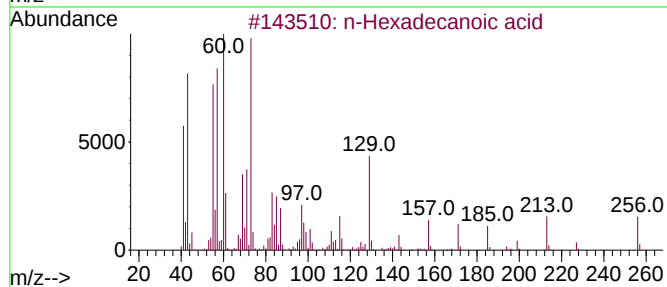
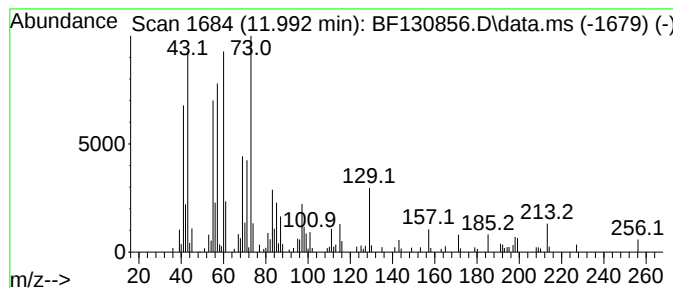
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.992	5.27 ng	162650	Phenanthrene-d10		11.475	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	93
3	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	83
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
5	Pentadecanoic acid		242	C15H30O2	001002-84-2	80



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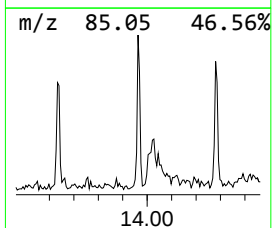
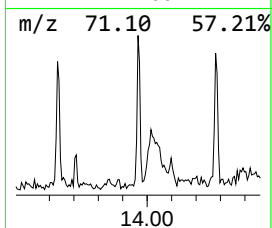
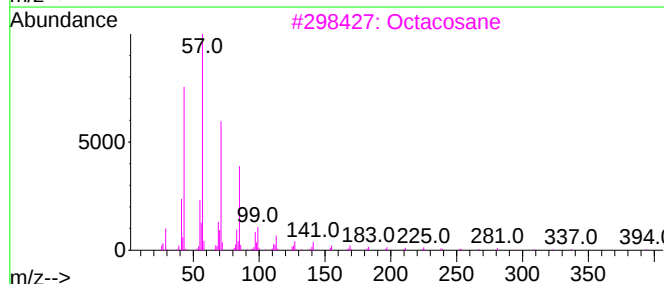
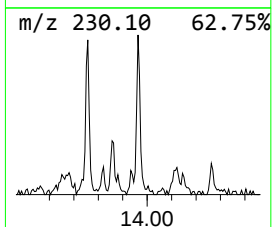
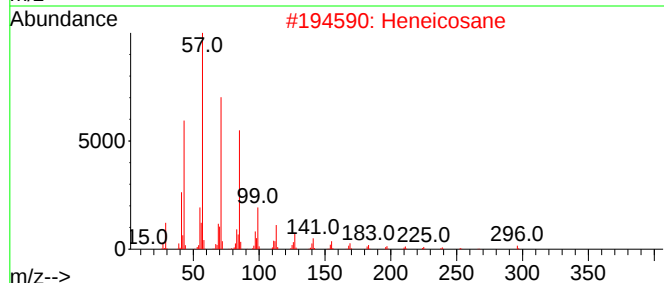
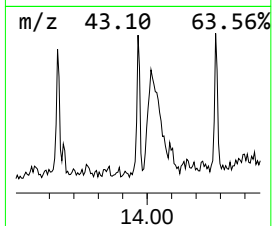
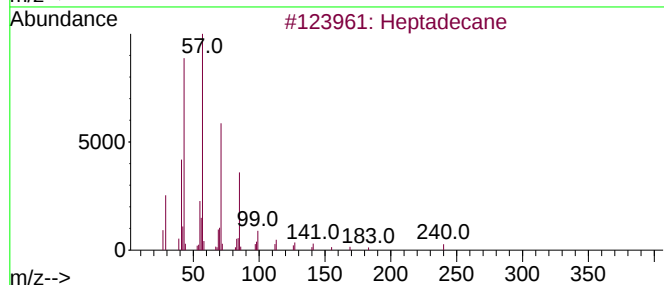
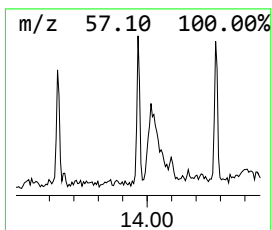
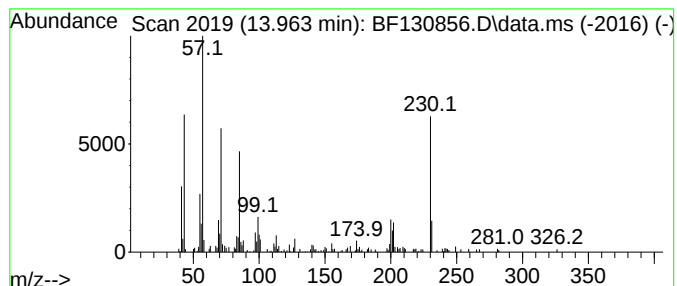
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.963	2.38 ng	78009	Chrysene-d12	14.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	90
2			Heneicosane	296	C21H44	000629-94-7	55
3			Octacosane	394	C28H58	000630-02-4	50
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	49
5			Nonadecane	268	C19H40	000629-92-5	49



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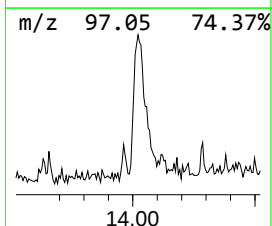
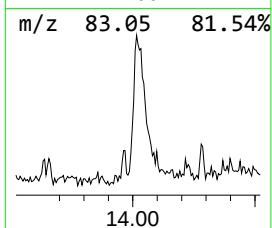
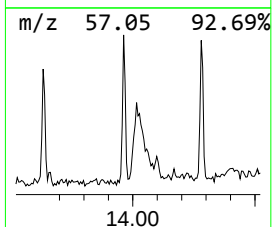
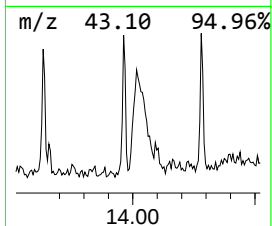
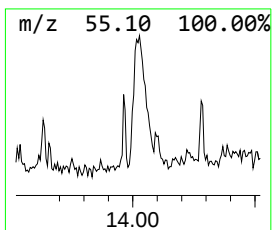
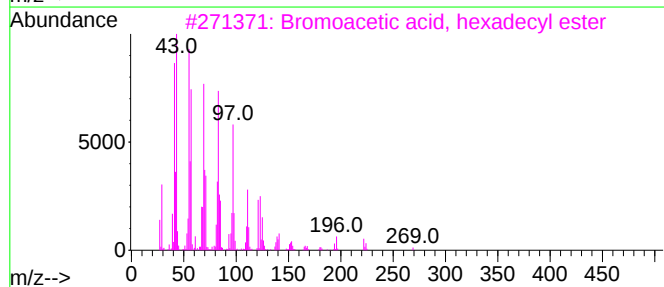
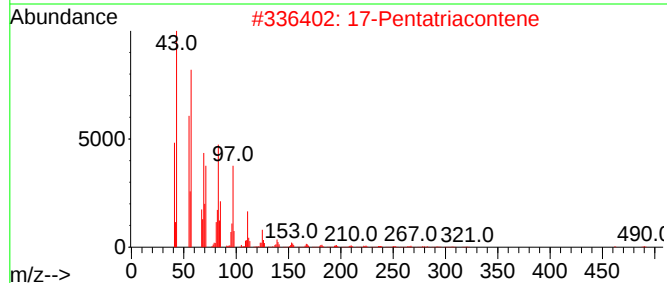
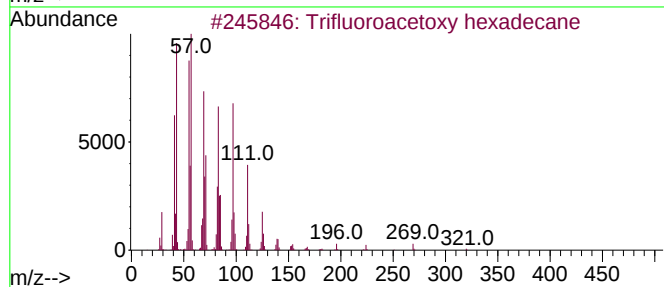
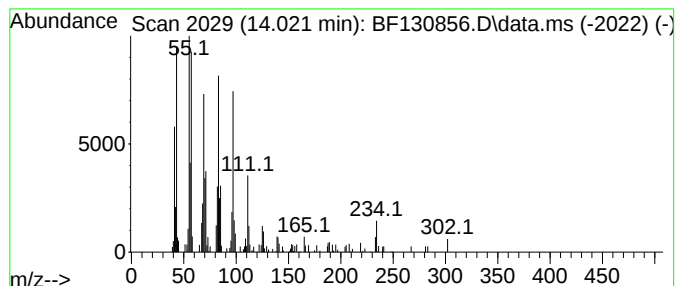
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.021	6.99 ng	228708	Chrysene-d12	14.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2			17-Pentatriacontene	491	C35H70	006971-40-0	90
3			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
4			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	90
5			1-Docosene	308	C22H44	001599-67-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130856.D
Acq On : 29 Oct 2022 14:43
Operator : CG\JU
Sample : N5332-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4-WC

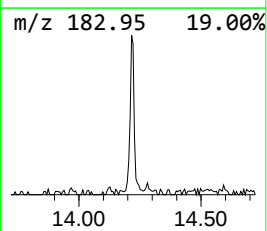
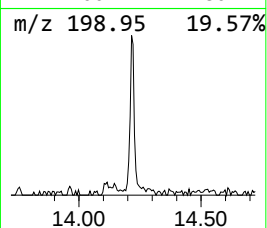
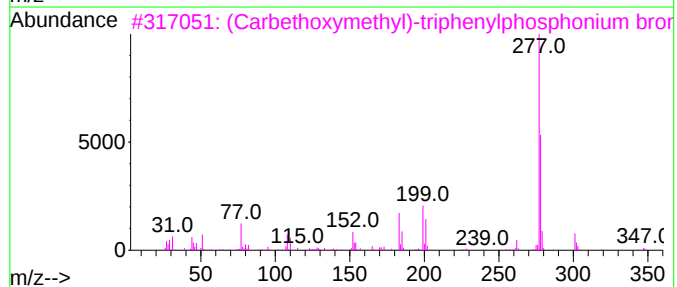
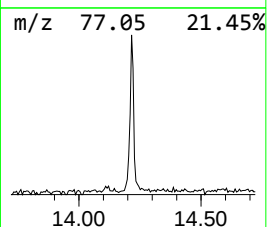
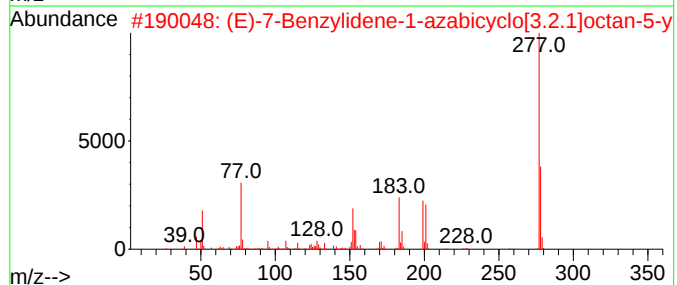
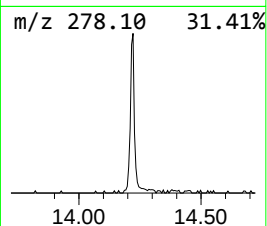
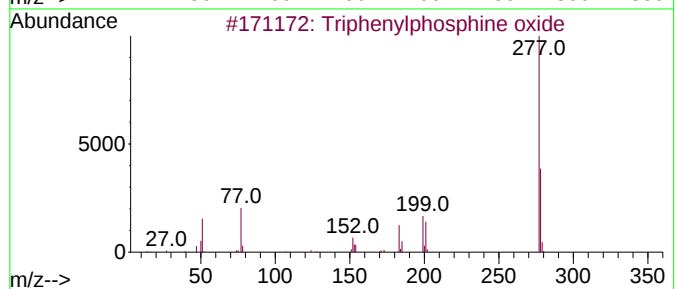
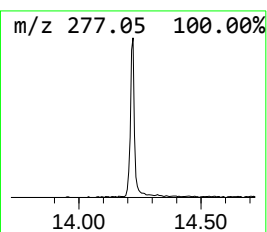
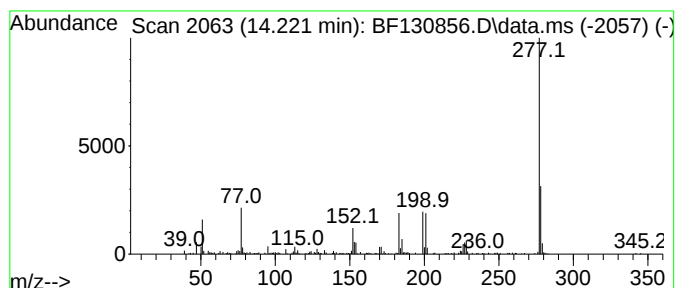
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	6.54 ng	214154	Chrysene-d12	14.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
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Operator : CG\JU
Sample : N5332-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

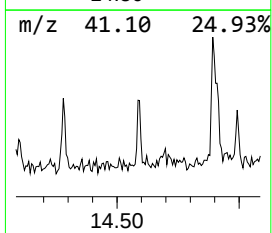
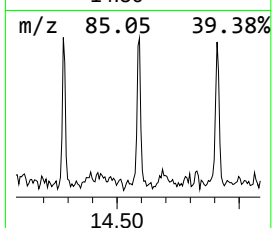
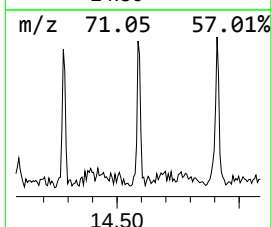
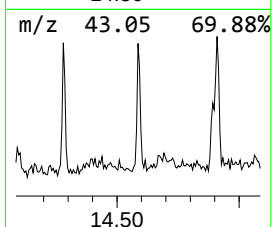
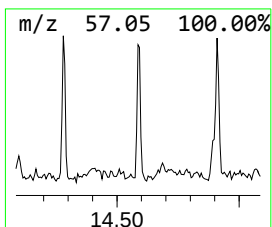
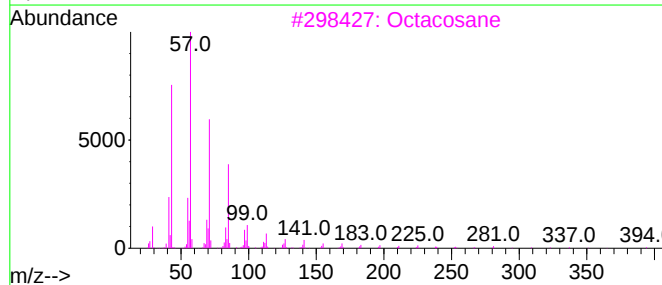
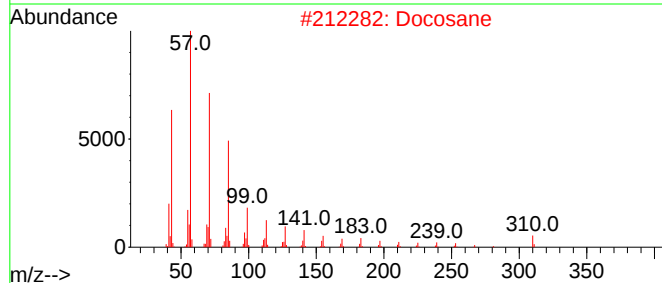
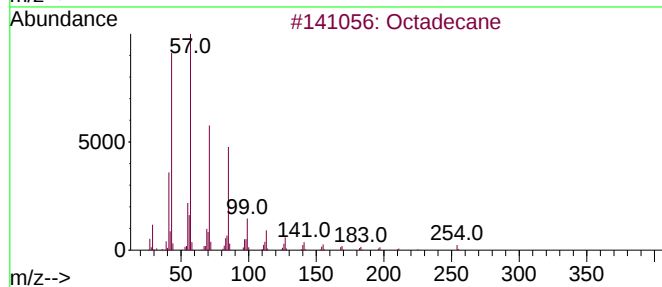
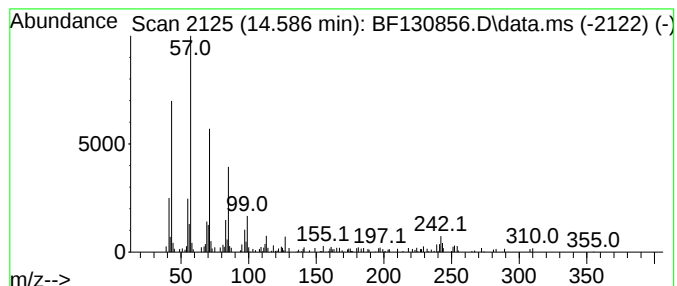
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ClientSampleId :
MH-4-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.586	2.17 ng	71115	Chrysene-d12		14.121	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	93
2	Docosane		310	C22H46	000629-97-0	93
3	Octacosane		394	C28H58	000630-02-4	90
4	Hexacosane		366	C26H54	000630-01-3	90
5	Octacosane, 2-methyl-		408	C29H60	001560-98-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130856.D
Acq On : 29 Oct 2022 14:43
Operator : CG\JU
Sample : N5332-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4-WC

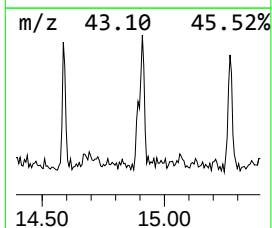
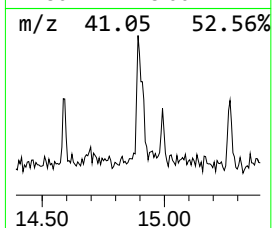
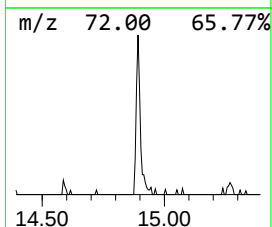
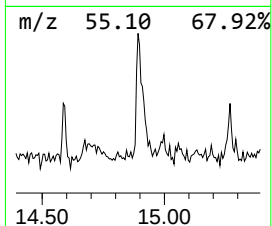
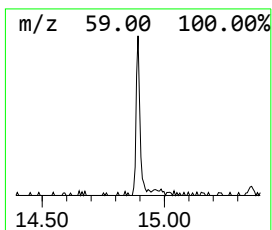
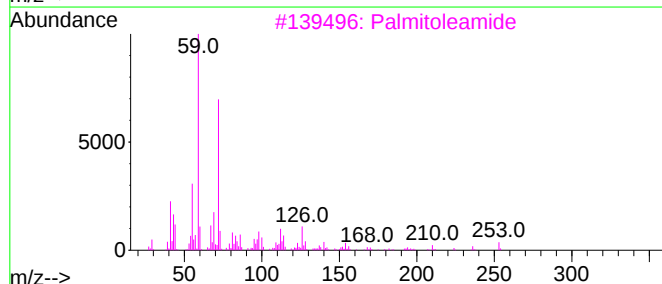
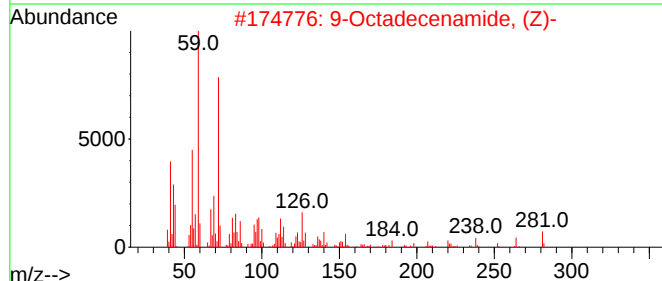
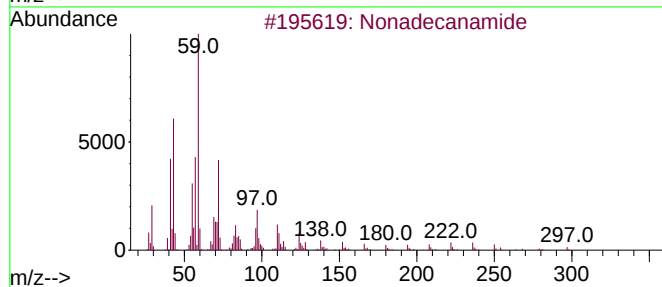
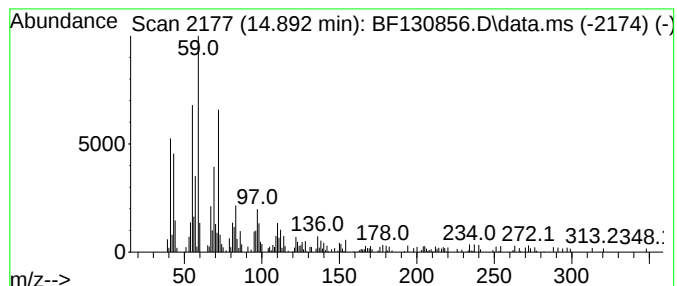
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Nonadecanamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.892	5.13 ng	104835	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecanamide	297	C19H39NO	058185-32-3	74
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
3			Palmitoleamide	253	C16H31NO	106010-22-4	64
4			cis-Vaccenic acid	282	C18H34O2	000506-17-2	53
5			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130856.D
Acq On : 29 Oct 2022 14:43
Operator : CG\JU
Sample : N5332-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4-WC

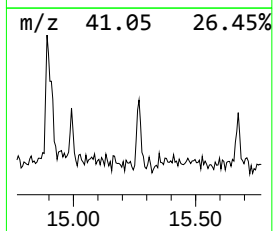
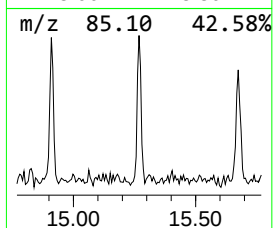
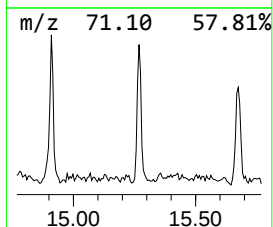
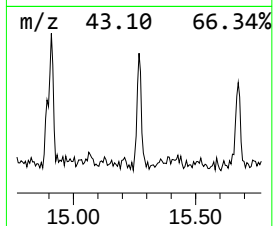
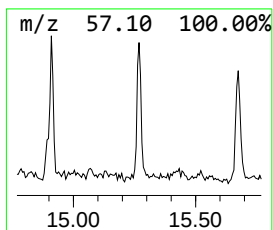
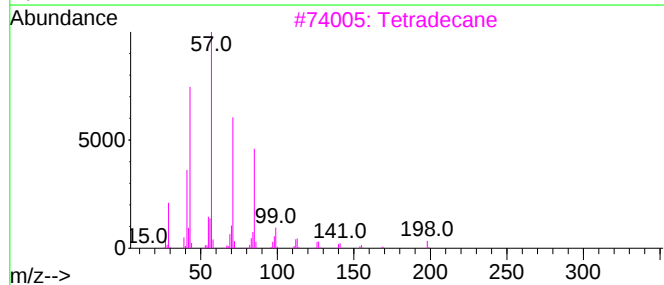
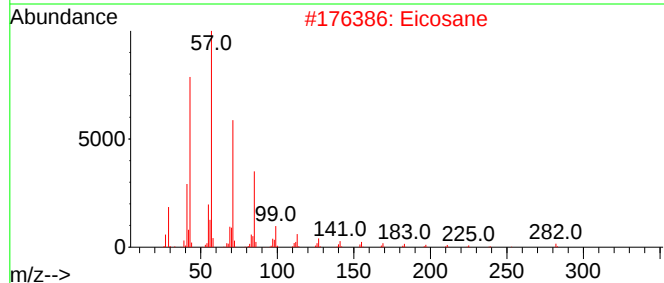
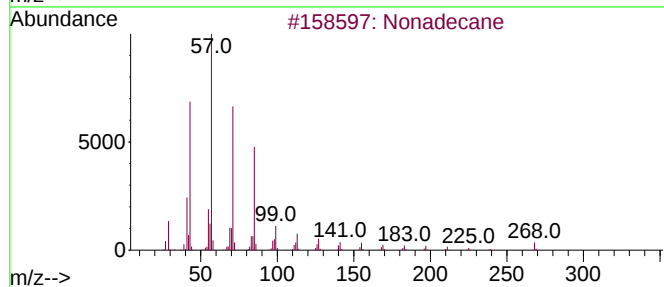
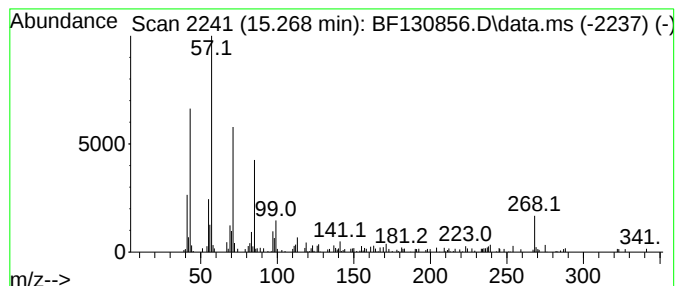
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.268	3.37 ng	68824	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	90
2			Eicosane	282	C20H42	000112-95-8	90
3			Tetradecane	198	C14H30	000629-59-4	89
4			Heneicosane	296	C21H44	000629-94-7	80
5			Octadecane	254	C18H38	000593-45-3	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130856.D
Acq On : 29 Oct 2022 14:43
Operator : CG\JU
Sample : N5332-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MH-4-WC

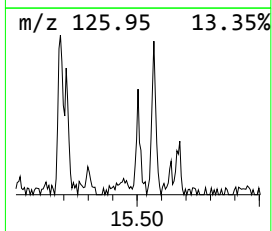
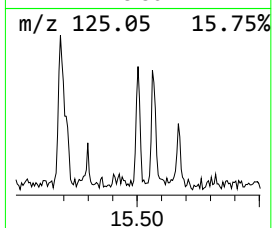
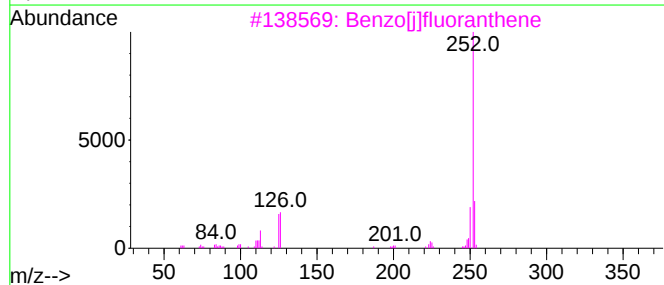
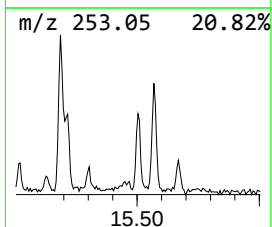
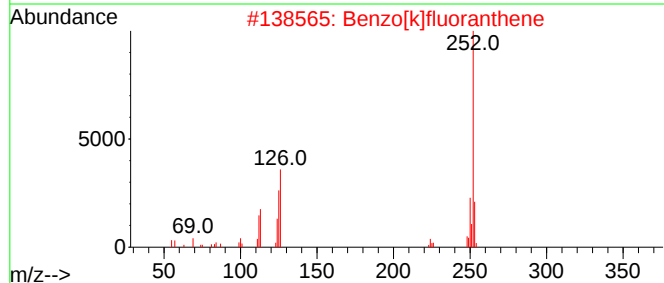
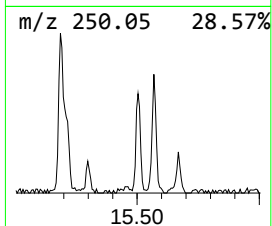
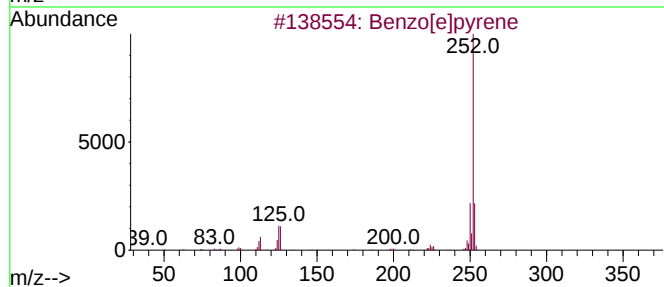
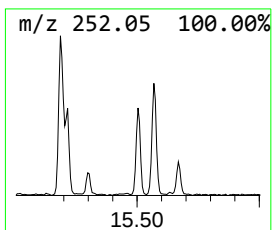
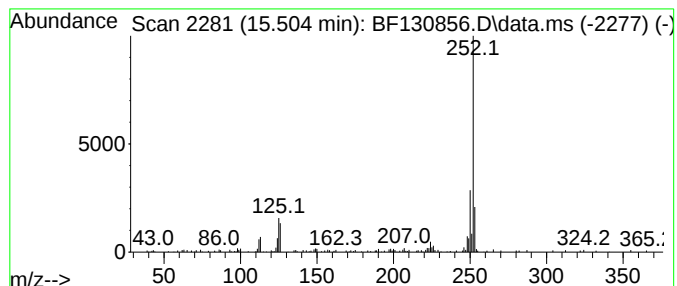
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.504	4.30 ng	87983	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	95
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	91
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130856.D
Acq On : 29 Oct 2022 14:43
Operator : CG\JU
Sample : N5332-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4-WC

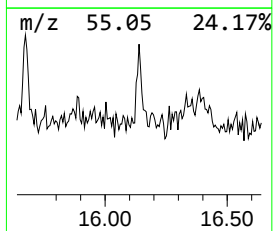
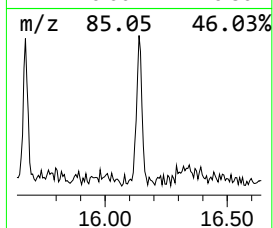
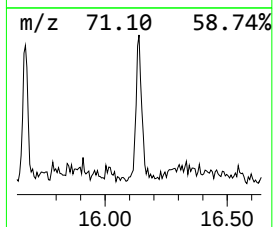
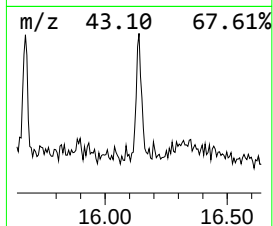
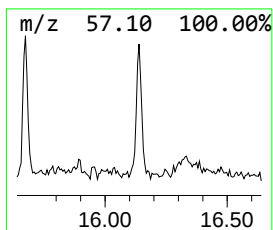
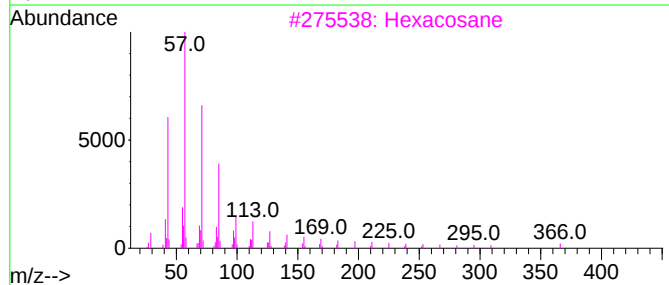
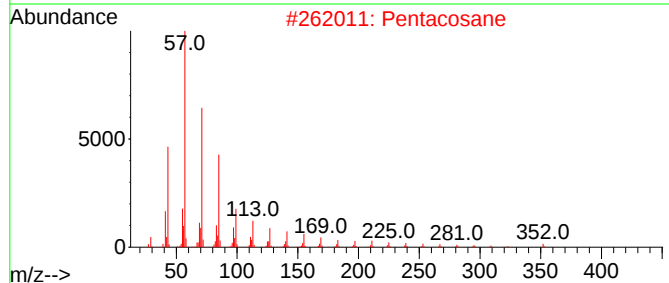
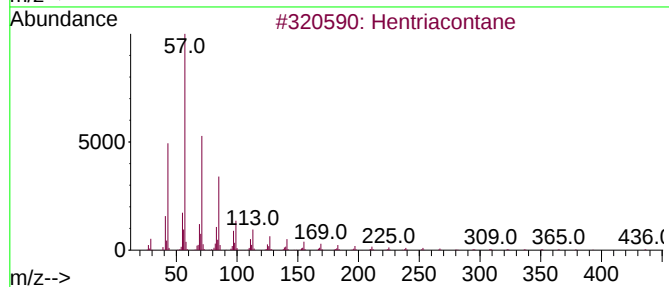
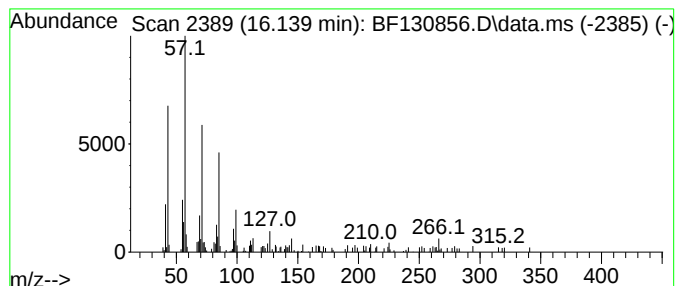
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.139	3.21 ng	65726	Perylene-d12	15.639

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	86
2		Pentacosane	352	C25H52	000629-99-2	86
3		Hexacosane	366	C26H54	000630-01-3	86
4		5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	86
5		Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130856.D
Acq On : 29 Oct 2022 14:43
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4-WC

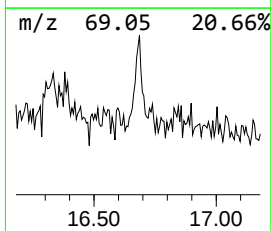
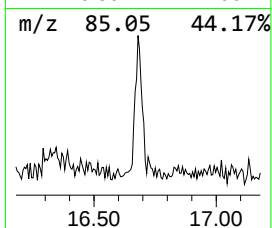
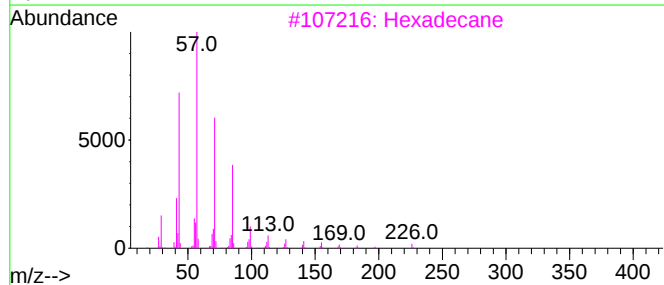
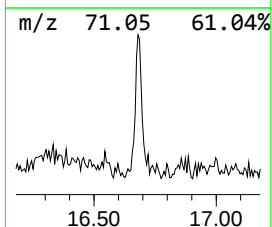
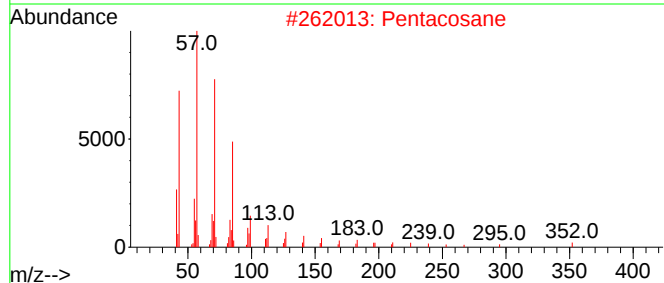
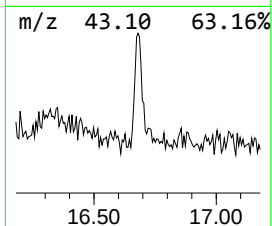
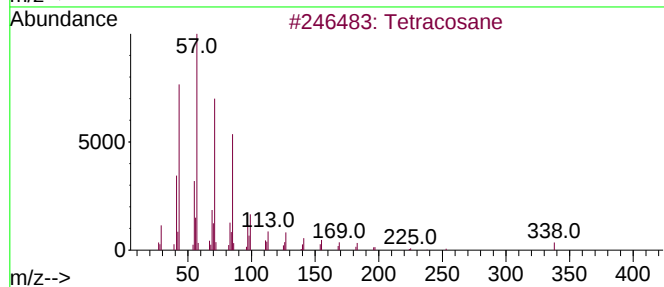
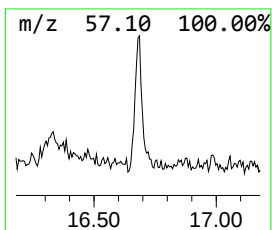
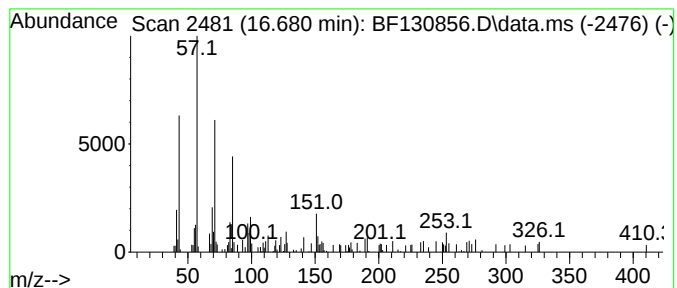
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.680	3.26 ng	66719	Perylene-d12	15.639

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	64
2		Pentacosane	352	C25H52	000629-99-2	64
3		Hexadecane	226	C16H34	000544-76-3	64
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	58
5		Tricosane	324	C23H48	000638-67-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130856.D
Acq On : 29 Oct 2022 14:43
Operator : CG\JU
Sample : N5332-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.275	26.6	ng	728745	1	6.940	547928	20.0
2-Pentanone, 4-...	5.175	16.3	ng	446074	1	6.940	547928	20.0
n-Hexadecanoic ...	11.992	5.3	ng	162650	4	11.475	616914	20.0
Heptadecane	13.963	2.4	ng	78009	5	14.121	654842	20.0
Trifluoroacetox...	14.021	7.0	ng	228708	5	14.121	654842	20.0
Triphenylphosph...	14.221	6.5	ng	214154	5	14.121	654842	20.0
Octadecane	14.586	2.2	ng	71115	5	14.121	654842	20.0
Nonadecanamide	14.892	5.1	ng	104835	6	15.639	409058	20.0
Nonadecane	15.268	3.4	ng	68824	6	15.639	409058	20.0
Benzo[e]pyrene	15.504	4.3	ng	87983	6	15.639	409058	20.0
Hentriacontane	16.139	3.2	ng	65726	6	15.639	409058	20.0
Tetracosane	16.680	3.3	ng	66719	6	15.639	409058	20.0