

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100518\
 Data File : BF109630.D
 Acq On : 6 Oct 2018 1:17
 Operator : JU/SJ
 Sample : J5263-09
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID18-COMP-100318

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-BF092218.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	4.899	475	478	490	rVB	46565	62744	3.67%	0.377%
2	5.328	547	551	565	rBV	1307510	1494993	87.33%	8.975%
3	6.351	721	725	742	rBV	1421582	1711434	99.97%	10.274%
4	6.475	742	746	769	rVB	1774596	1711914	100.00%	10.277%
5	6.704	781	785	794	rBV	447778	504546	29.47%	3.029%
6	6.775	794	797	807	rVB2	14009	26877	1.57%	0.161%
7	6.857	807	811	838	rBV	1434860	1282802	74.93%	7.701%
8	7.263	876	880	909	rBV	968868	1069144	62.45%	6.418%
9	7.981	999	1002	1019	rBV	627580	626844	36.62%	3.763%
10	9.057	1181	1185	1199	rBV	1665955	1539804	89.95%	9.244%
11	9.451	1249	1252	1260	rBV	142405	137037	8.00%	0.823%
12	9.728	1295	1299	1314	rBV2	625878	597406	34.90%	3.586%
13	10.516	1429	1433	1451	rBV	799176	848333	49.55%	5.093%
14	11.204	1547	1550	1553	rBV	457382	487117	28.45%	2.924%
15	11.286	1560	1564	1568	rVB2	13083	17674	1.03%	0.106%
16	11.745	1638	1642	1647	rBV2	67783	75795	4.43%	0.455%
17	12.304	1733	1737	1741	rVB6	13802	18086	1.06%	0.109%
18	12.416	1752	1756	1762	rBV	110426	121517	7.10%	0.730%
19	12.639	1788	1794	1797	rBV2	105951	115595	6.75%	0.694%
20	12.786	1815	1819	1827	rVB	1445087	1245640	72.76%	7.478%
21	12.857	1827	1831	1837	rBV4	11387	20016	1.17%	0.120%
22	12.969	1847	1850	1853	rVB2	20001	21136	1.23%	0.127%
23	13.027	1857	1860	1864	rVB2	20484	24452	1.43%	0.147%
24	13.369	1912	1918	1920	rBV2	35474	37130	2.17%	0.223%
25	13.580	1950	1954	1957	rBV3	13354	20241	1.18%	0.122%
26	13.692	1969	1973	1980	rBV2	103450	146652	8.57%	0.880%
27	13.833	1990	1997	2000	rBV	691207	725280	42.37%	4.354%
28	14.010	2024	2027	2032	rVB	71574	66528	3.89%	0.399%
29	14.316	2075	2079	2082	rBV	99709	101413	5.92%	0.609%
30	14.604	2125	2128	2132	rBV	159426	152329	8.90%	0.914%
31	14.674	2136	2140	2143	rBV	101615	94662	5.53%	0.568%
32	14.845	2164	2169	2177	rBV	62695	134478	7.86%	0.807%
33	14.916	2177	2181	2192	rVB2	174613	219895	12.84%	1.320%
34	15.121	2212	2216	2222	rVB	32321	53681	3.14%	0.322%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.174	2222	2225	2230	rVB	48522	60495	3.53%	0.363%
36	15.233	2230	2235	2238	rBV	391078	493190	28.81%	2.961%
37	15.268	2238	2241	2248	rVB	176902	215301	12.58%	1.293%
38	15.668	2304	2309	2315	rVB	110236	160118	9.35%	0.961%
39	16.121	2381	2386	2394	rVB	74706	124913	7.30%	0.750%
40	16.586	2461	2465	2472	rVB2	13157	26645	1.56%	0.160%
41	16.657	2472	2477	2484	rBV2	29348	63527	3.71%	0.381%

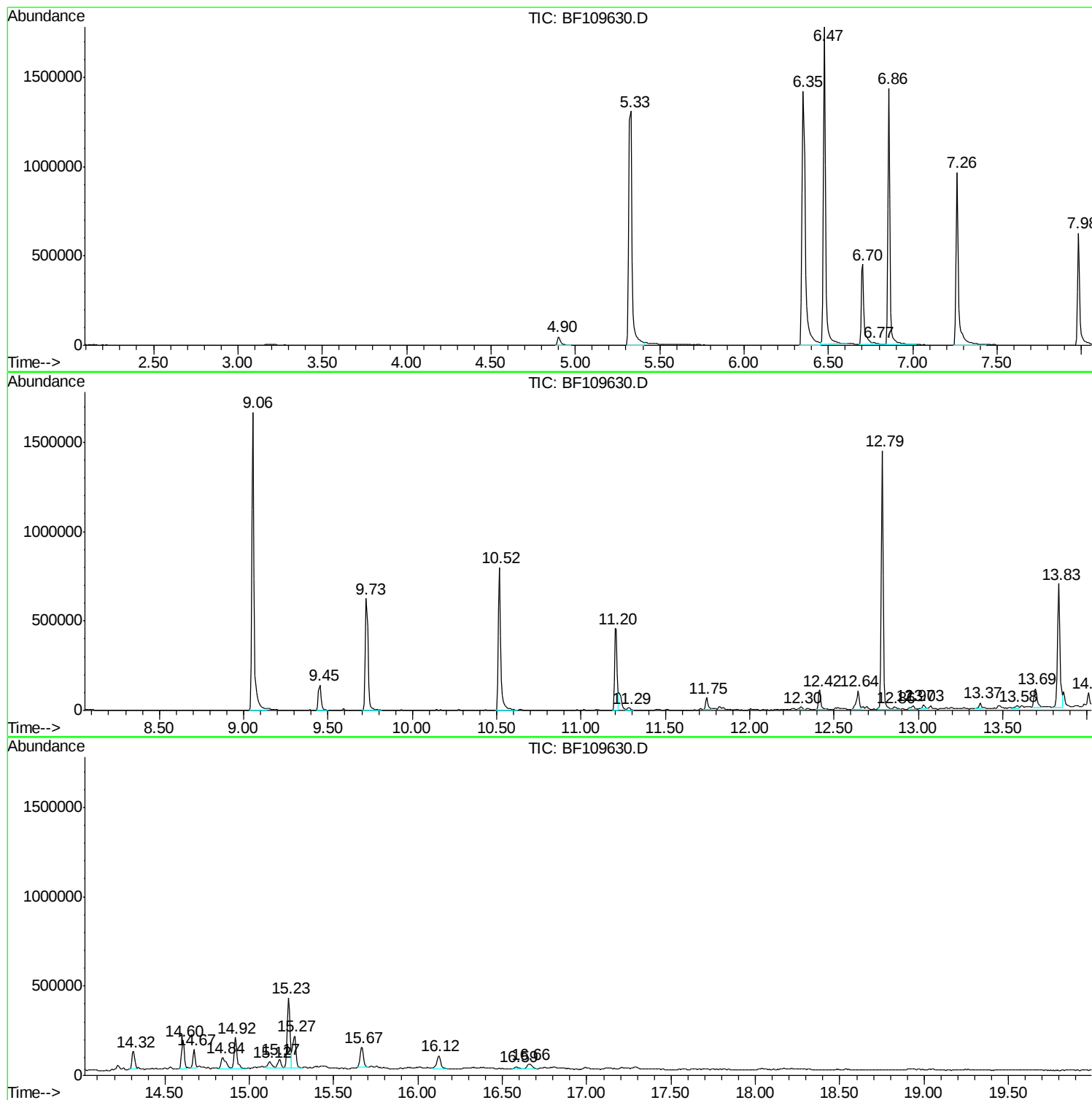
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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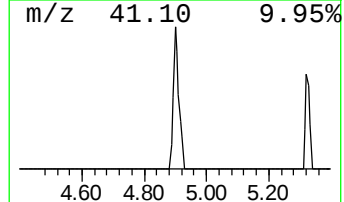
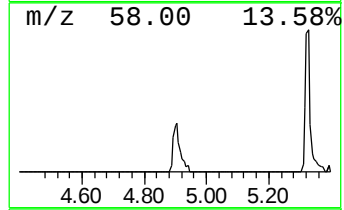
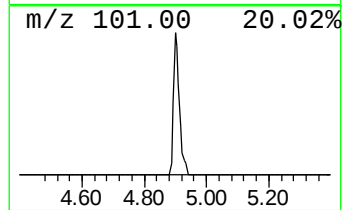
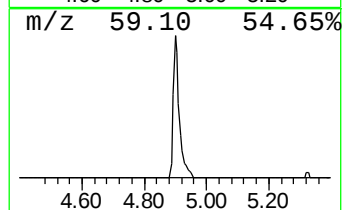
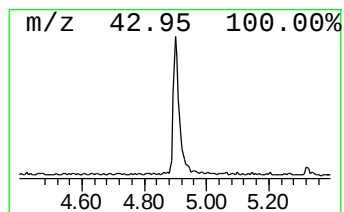
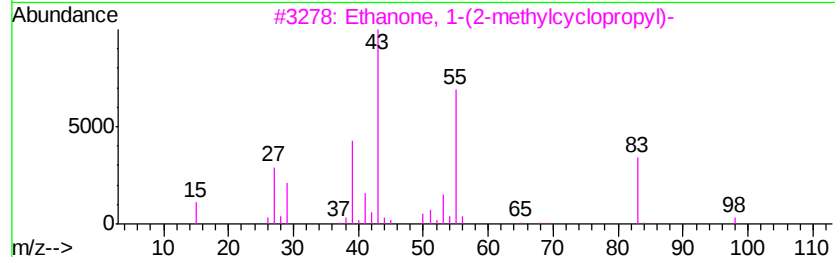
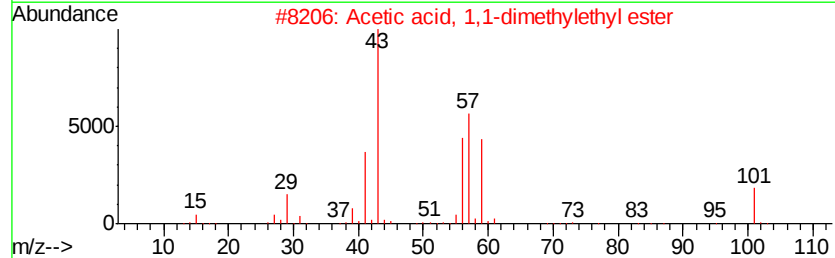
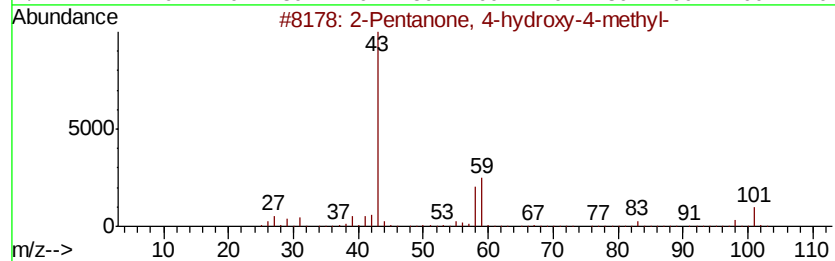
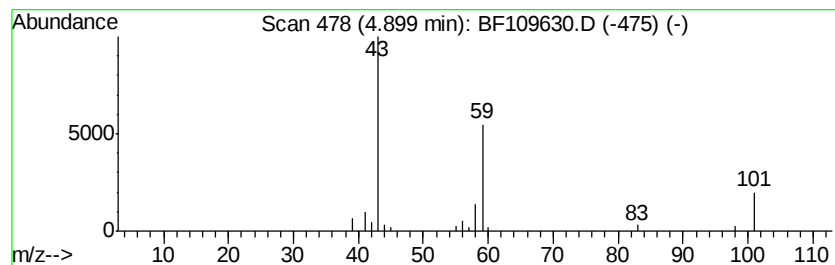
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.49 ng	62744	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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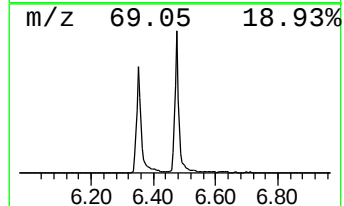
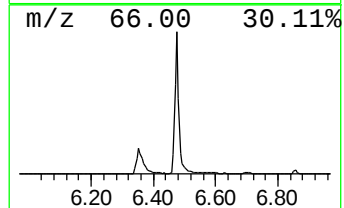
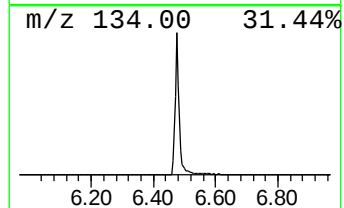
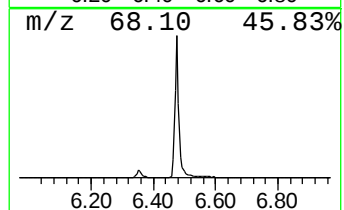
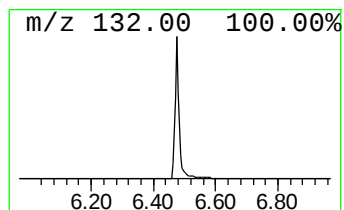
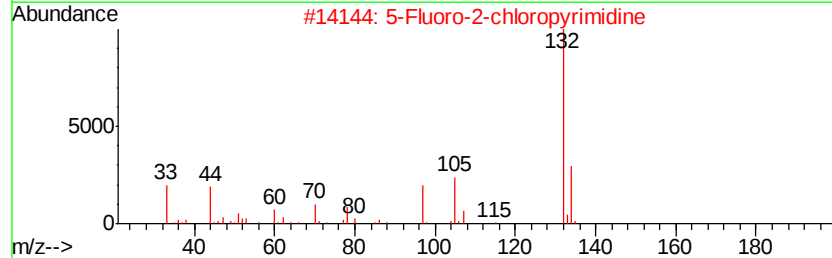
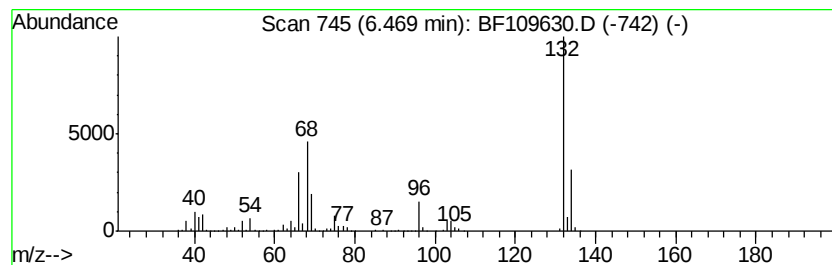
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	67.86 ng	1711910	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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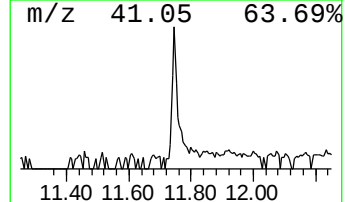
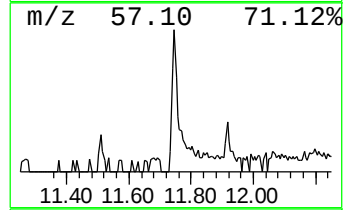
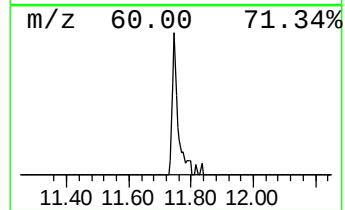
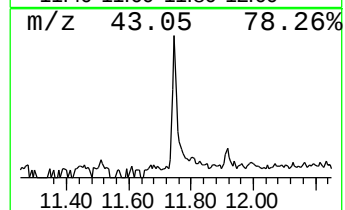
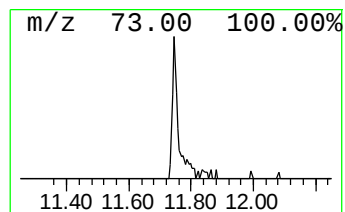
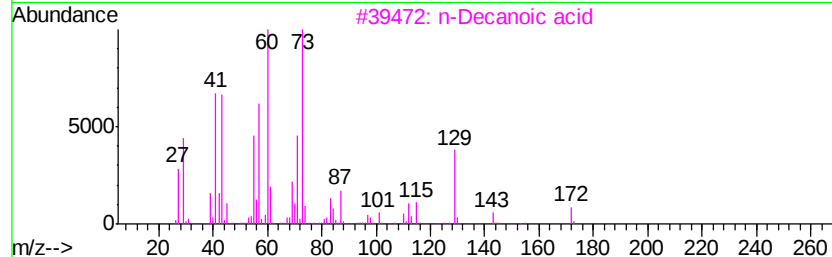
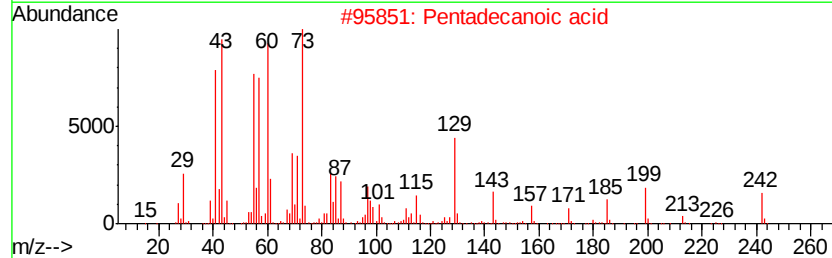
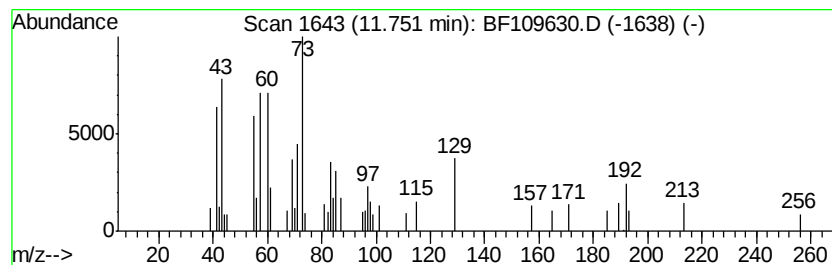
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	3.11 ng	75795	Phenanthrene-d10	11.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3		n-Decanoic acid	172	C10H20O2	000334-48-5	59
4		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



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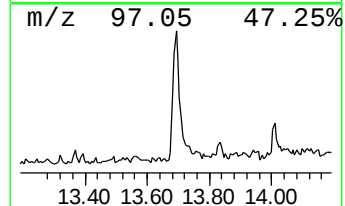
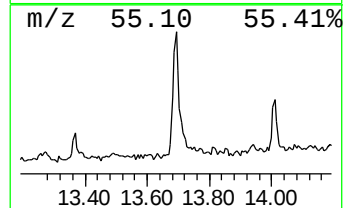
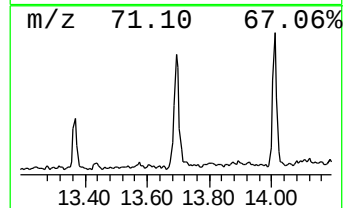
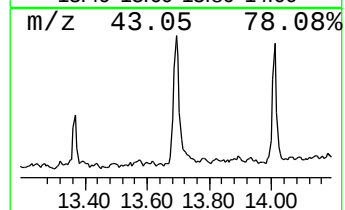
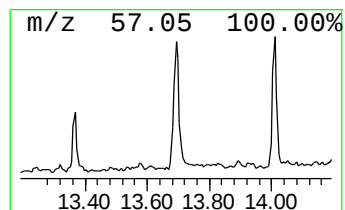
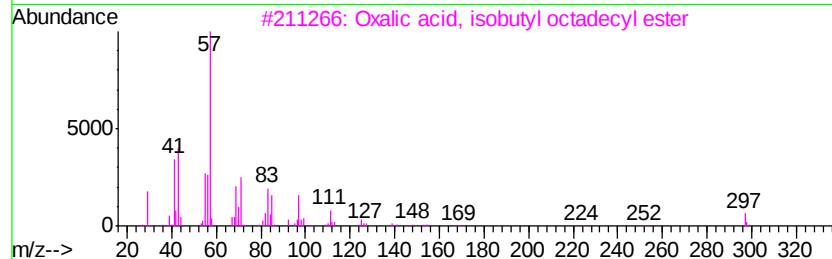
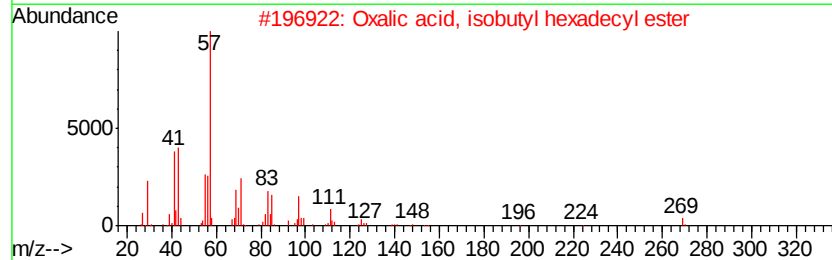
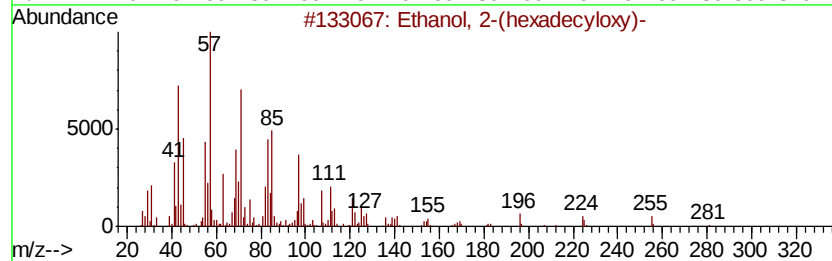
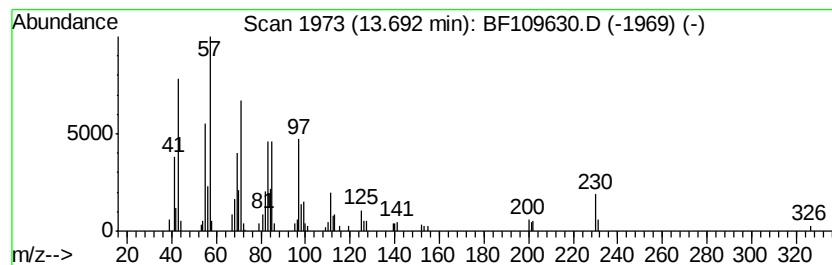
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(hexadecyloxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.69	4.04 ng	146652	Chrysene-d12	13.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	87
2		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	83
3		Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	83
4		Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	80
5		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	72



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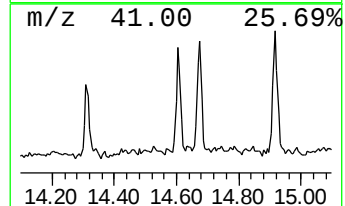
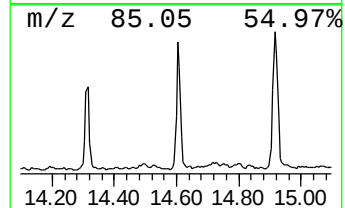
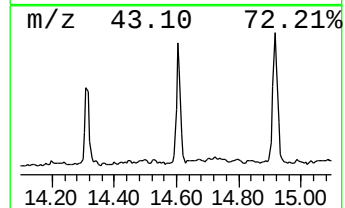
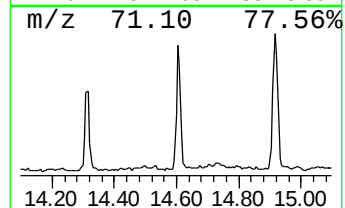
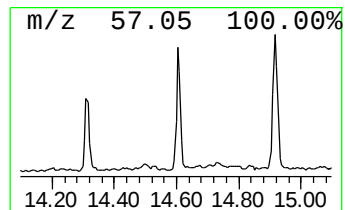
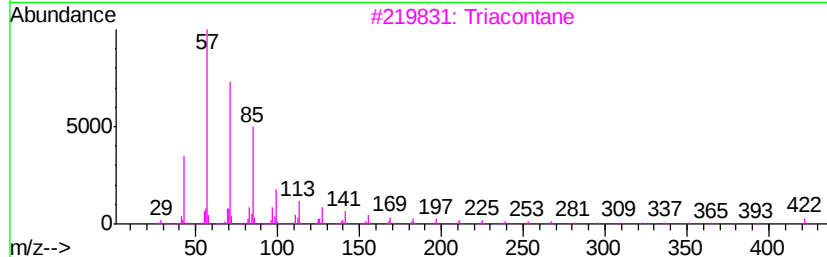
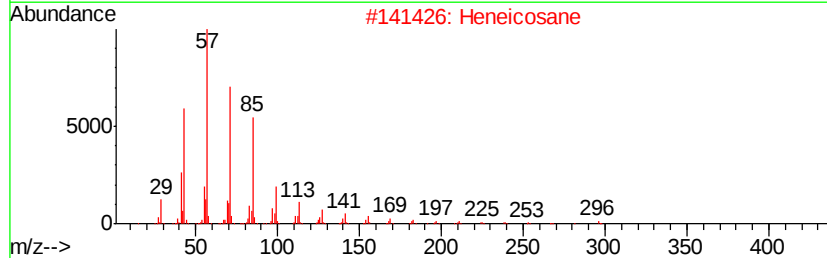
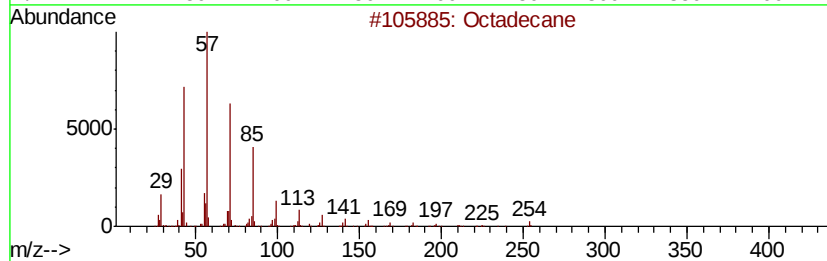
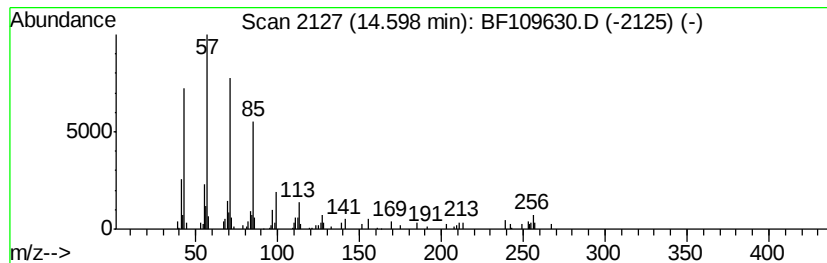
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	6.18 ng	152329	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	95
2		Heneicosane	296	C21H44	000629-94-7	91
3		Triacontane	422	C30H62	000638-68-6	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Eicosane, 2-methyl-	296	C21H44	001560-84-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109630.D
Acq On : 6 Oct 2018 1:17
Operator : JU/SJ
Sample : J5263-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID18-COMP-100318

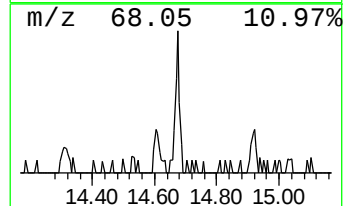
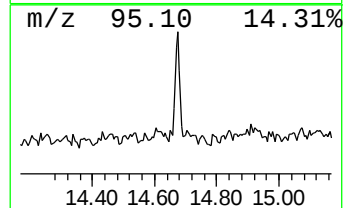
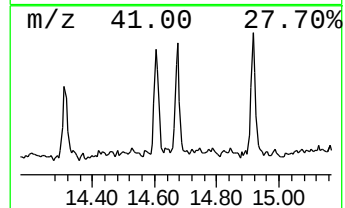
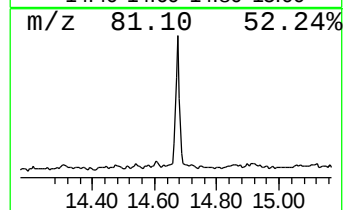
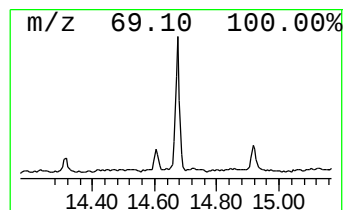
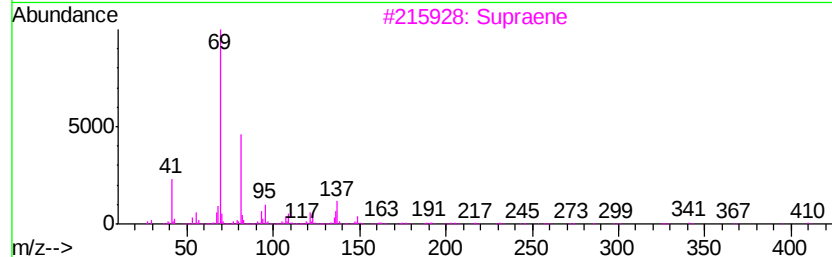
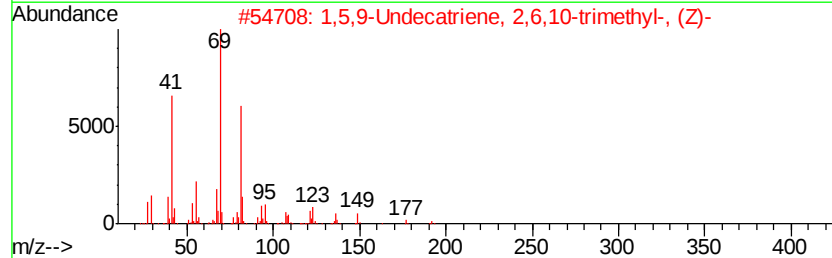
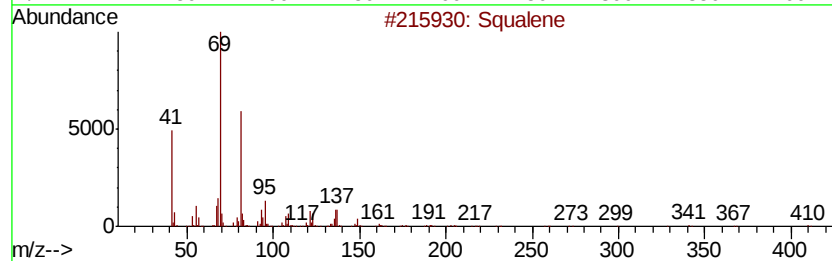
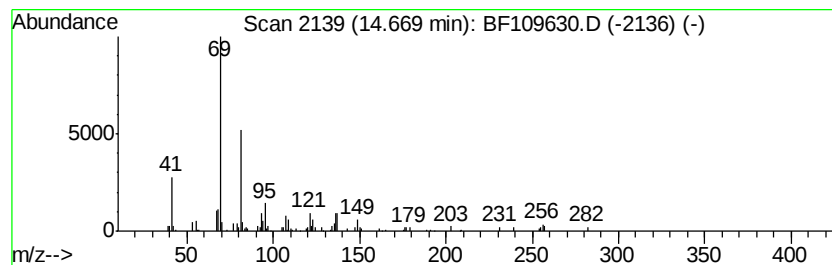
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	3.84 ng	94662	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
3		Supraene	410	C30H50	007683-64-9	80
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72



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 Misc :
 ALS Vial : 16 Sample Multiplier: 1

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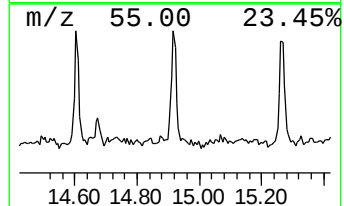
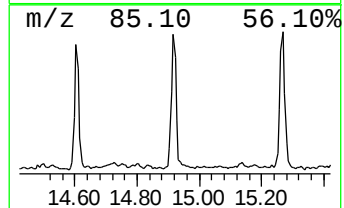
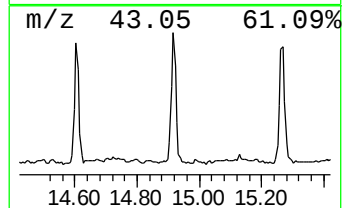
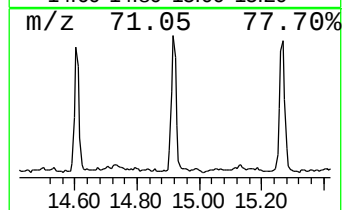
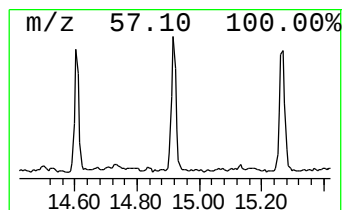
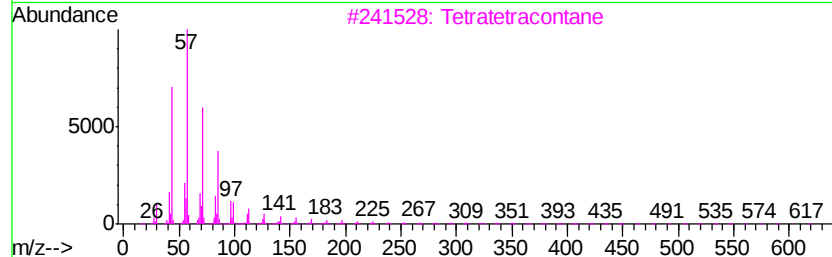
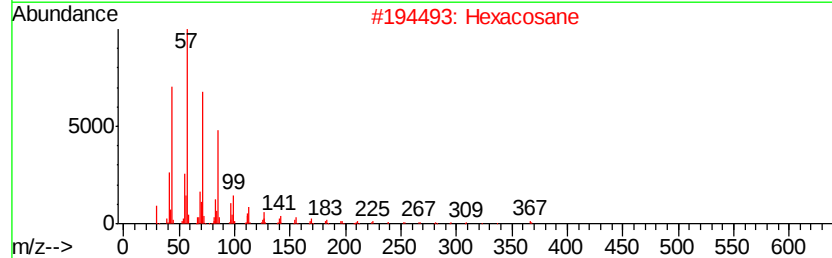
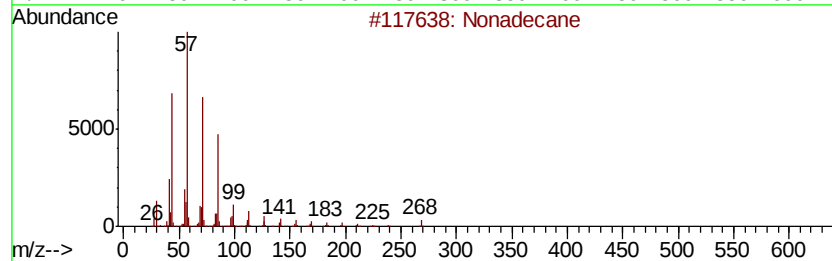
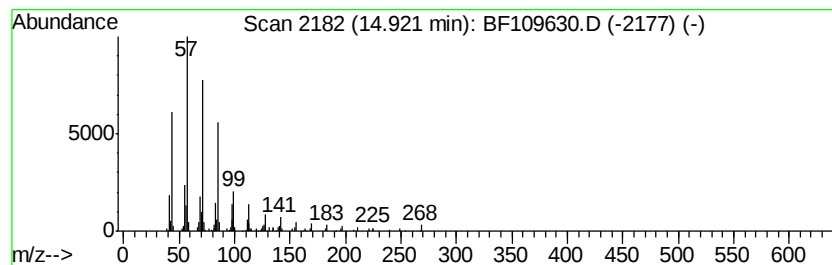
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	8.92 ng	219895	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	98
2	Hexacosane		366	C26H54	000630-01-3	93
3	Tetratetracontane		619	C44H90	007098-22-8	90
4	2-methyloctacosane		408	C29H60	1000376-72-8	90
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	90



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Data File : BF109630.D
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Sample : J5263-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID18-COMP-100318

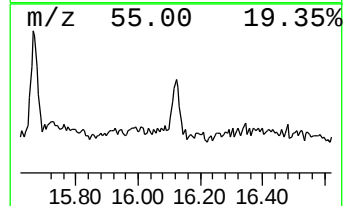
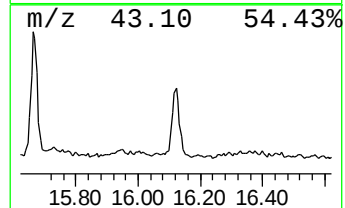
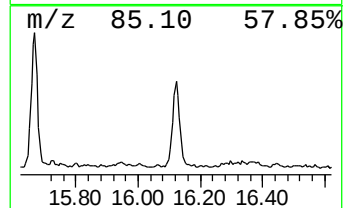
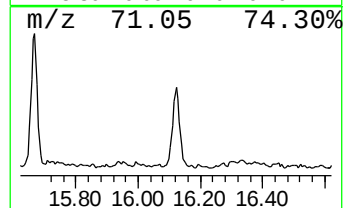
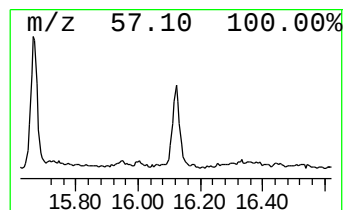
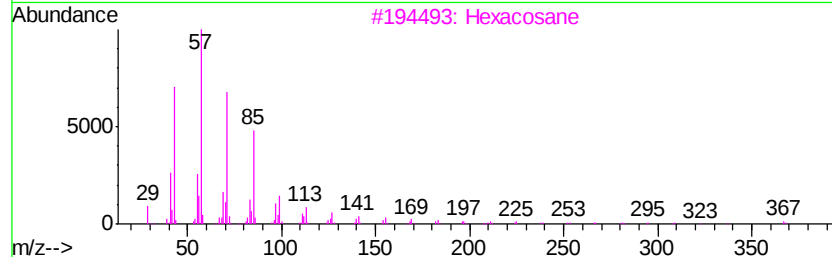
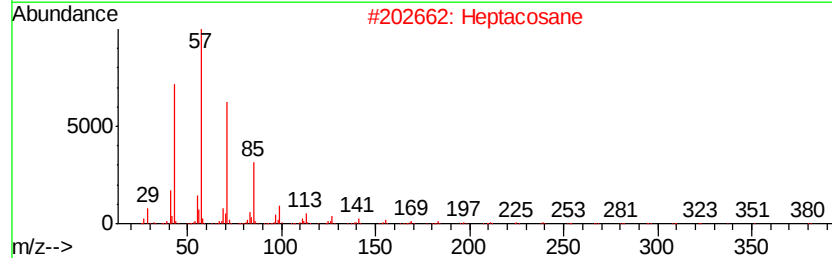
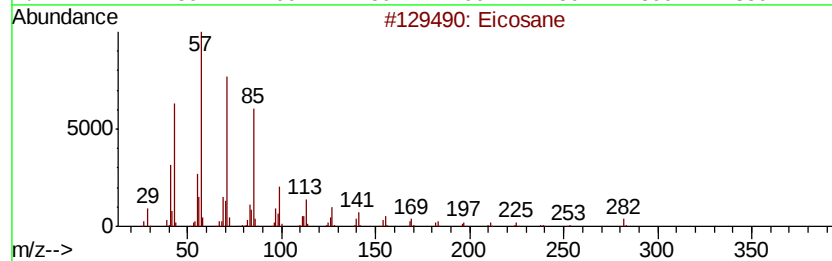
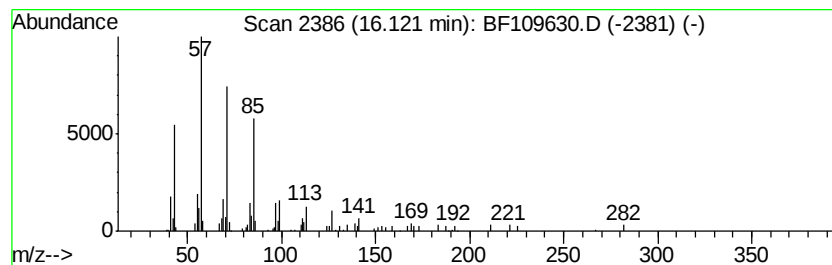
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	5.07 ng	124913	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	95
2		Heptacosane	380	C27H56	000593-49-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
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 Operator : JU/SJ
 Sample : J5263-09
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID18-COMP-100318

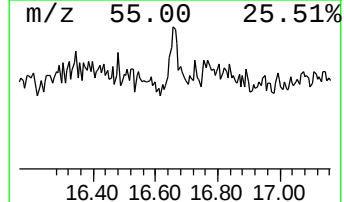
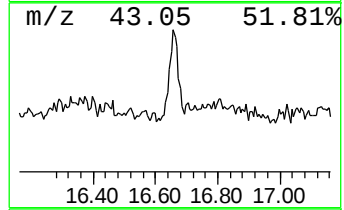
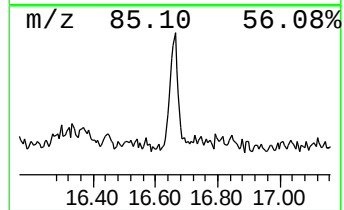
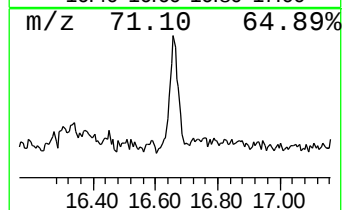
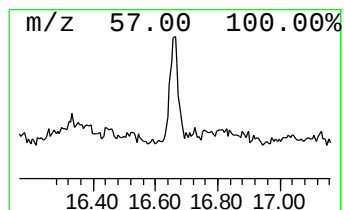
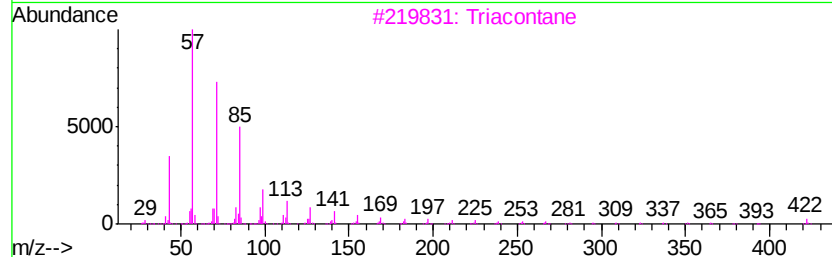
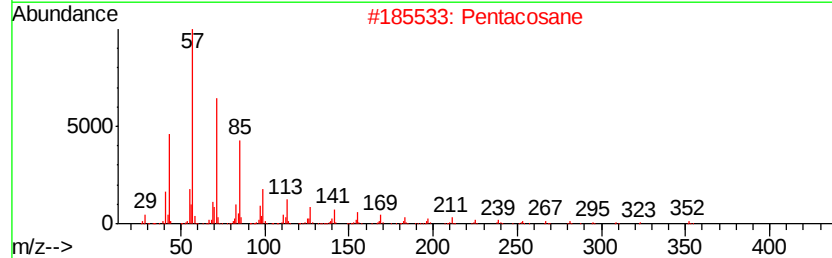
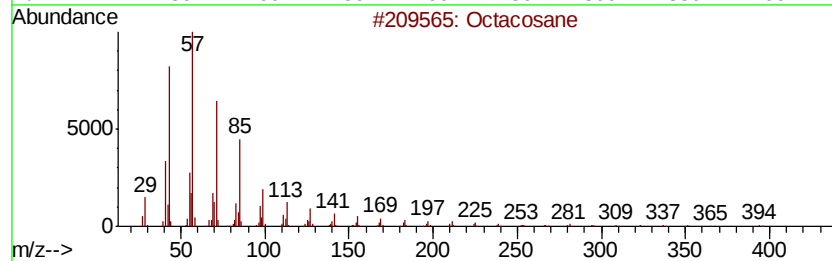
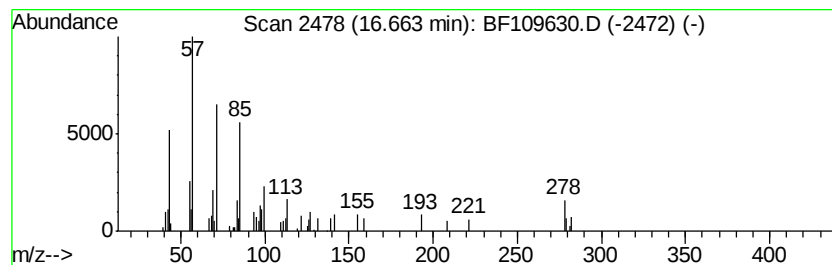
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 13 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	2.58 ng	63527	Perylene-d12	15.23

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Pentacosane	352	C25H52	000629-99-2	87
3			Triacontane	422	C30H62	000638-68-6	86
4			Heneicosane	296	C21H44	000629-94-7	83
5			Tetratetracontane	619	C44H90	007098-22-8	83



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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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
2-Pentanone, 4-hy...	4.90	2.5	ng	62744	1	6.70	504546	20.0
unknown6.47	6.47	67.9	ng	1711910	1	6.70	504546	20.0
n-Hexadecanoic acid	11.75	3.1	ng	75795	4	11.21	487117	20.0
Ethanol, 2-(hexad...	13.69	4.0	ng	146652	5	13.83	725280	20.0
Octadecane	14.60	6.2	ng	152329	6	15.23	493190	20.0
Squalene	14.67	3.8	ng	94662	6	15.23	493190	20.0
Nonadecane	14.92	8.9	ng	219895	6	15.23	493190	20.0
Eicosane	16.12	5.1	ng	124913	6	15.23	493190	20.0
Octacosane	16.66	2.6	ng	63527	6	15.23	493190	20.0