

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
 Data File : BF097137.D
 Acq On : 27 Jul 2017 22:05
 Operator : SJ/JU
 Sample : I4424-04 2X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AU-06-072417-B

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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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	3.198	217	223	231	rBV	34343	64908	2.85%	0.385%
2	4.616	460	464	477	rBV	119705	160916	7.07%	0.955%
3	5.081	540	543	561	rBV	1036534	1092675	48.00%	6.487%
4	6.145	720	724	736	rBV	1182215	1184715	52.05%	7.034%
5	6.257	739	743	751	rVB	1227145	1066741	46.86%	6.333%
6	6.487	778	782	791	rBV	685707	623005	27.37%	3.699%
7	6.639	804	808	818	rBV	841468	741907	32.59%	4.405%
8	7.051	874	878	890	rBV	803844	704632	30.96%	4.184%
9	7.769	996	1000	1011	rBV	1063962	870905	38.26%	5.171%
10	8.845	1179	1183	1186	rBV	1181516	929522	40.84%	5.519%
11	9.245	1248	1251	1256	rBV	147852	110714	4.86%	0.657%
12	9.516	1293	1297	1300	rBV	939156	856814	37.64%	5.087%
13	9.945	1366	1370	1372	rBV	49684	45145	1.98%	0.268%
14	10.298	1426	1430	1435	rVB	556319	492798	21.65%	2.926%
15	10.439	1451	1454	1461	rBV	30757	39861	1.75%	0.237%
16	10.886	1522	1530	1533	rBV2	28462	28640	1.26%	0.170%
17	10.986	1543	1547	1551	rBV	766863	653472	28.71%	3.880%
18	11.410	1615	1619	1622	rVB	747747	632237	27.78%	3.754%
19	11.539	1636	1641	1644	rBV3	30786	30359	1.33%	0.180%
20	12.086	1730	1734	1736	rBV	2256466	2276226	100.00%	13.514%
21	12.110	1736	1738	1745	rVB	1909795	1657860	72.83%	9.843%
22	12.198	1749	1753	1756	rBV	396848	372785	16.38%	2.213%
23	12.227	1756	1758	1760	rVV2	29459	30975	1.36%	0.184%
24	12.245	1760	1761	1769	rVB3	23272	28169	1.24%	0.167%
25	12.416	1786	1790	1795	rVB2	29409	36243	1.59%	0.215%
26	12.568	1812	1816	1819	rVB	734582	629935	27.67%	3.740%
27	12.833	1856	1861	1864	rVB4	16568	26907	1.18%	0.160%
28	12.915	1872	1875	1877	rBV	36698	26955	1.18%	0.160%
29	13.339	1944	1947	1950	rBV4	23388	25515	1.12%	0.151%
30	13.486	1968	1972	1978	rVB3	40458	55185	2.42%	0.328%
31	13.580	1985	1988	1990	rBV	32372	34267	1.51%	0.203%
32	13.610	1990	1993	1997	rVB	597429	519240	22.81%	3.083%
33	14.115	2075	2079	2086	rBV2	31782	46603	2.05%	0.277%
34	14.404	2125	2128	2131	rBV	39215	36713	1.61%	0.218%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.692	2174	2177	2180	rBV2	39548	36194	1.59%	0.215%
36	14.957	2217	2222	2226	rBV	445680	514529	22.60%	3.055%
37	15.004	2228	2230	2234	rVB	47956	47685	2.09%	0.283%
38	15.362	2288	2291	2295	rBV3	29178	42364	1.86%	0.252%
39	15.774	2359	2361	2366	rVB	32768	41382	1.82%	0.246%
40	16.021	2402	2403	2407	rBV4	17271	27291	1.20%	0.162%

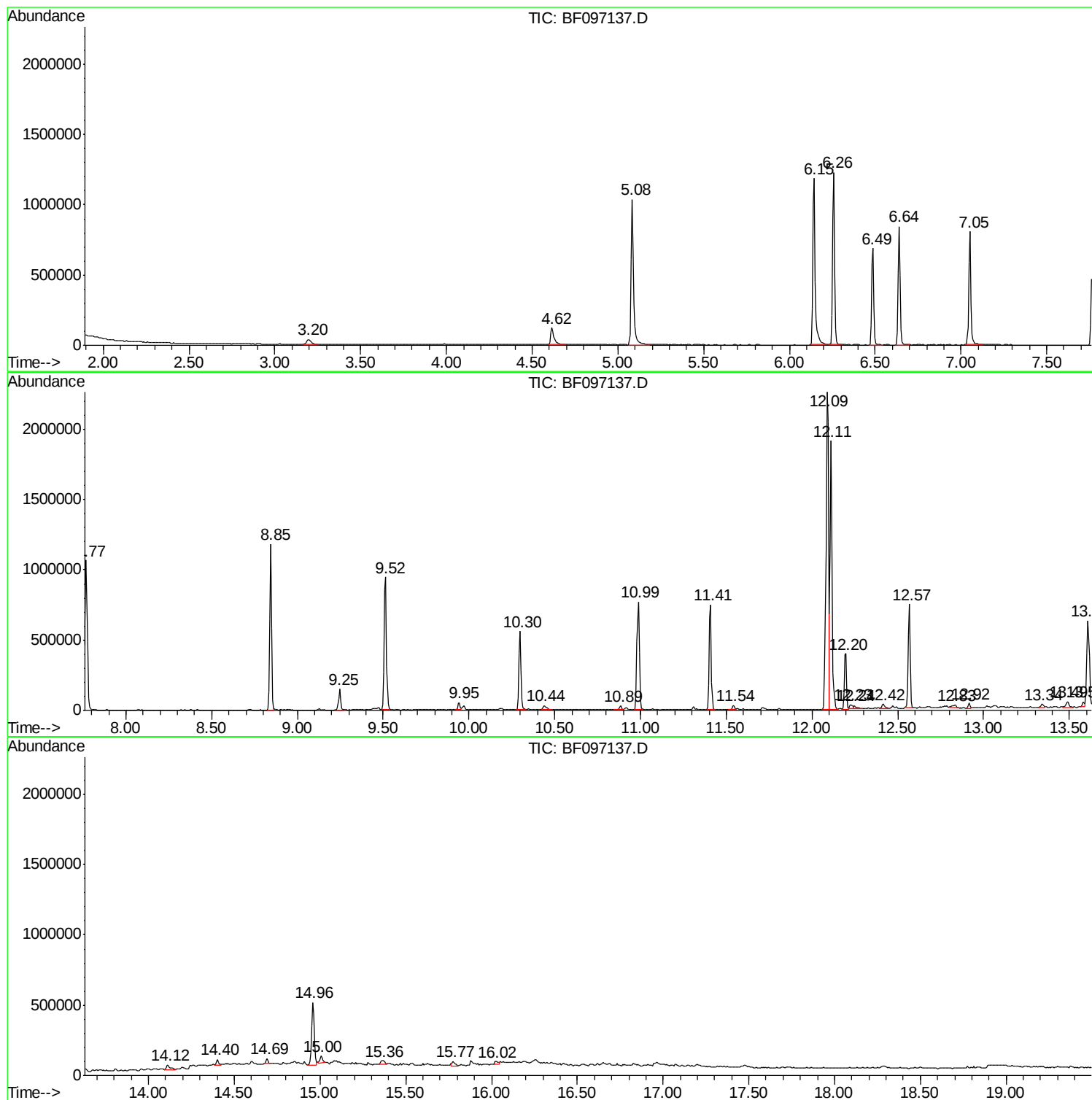
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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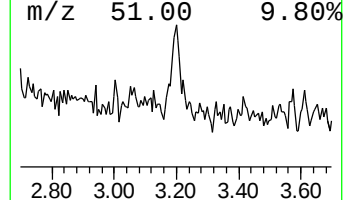
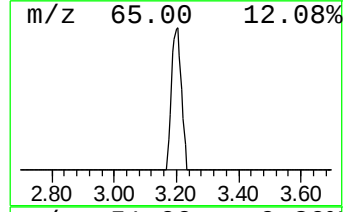
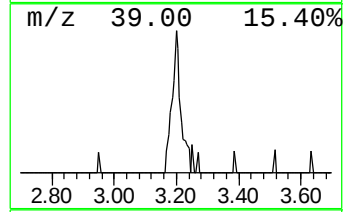
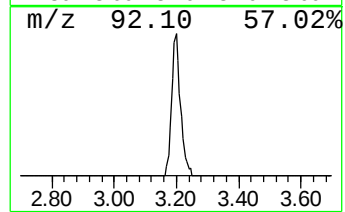
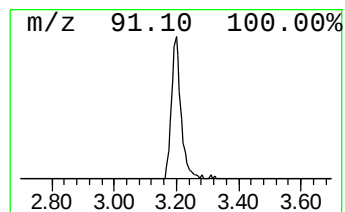
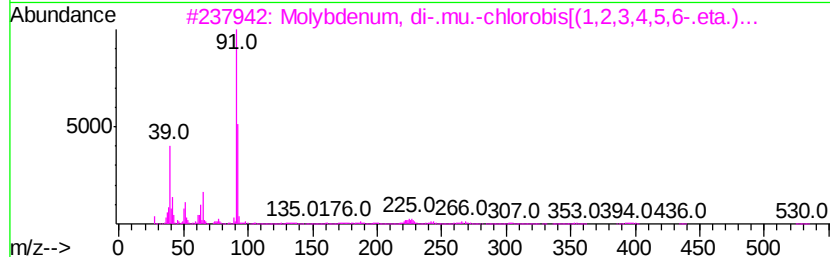
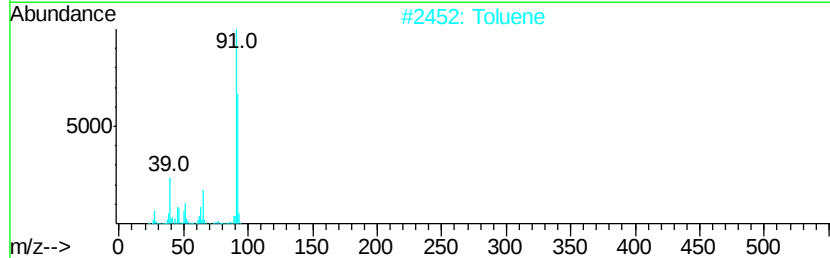
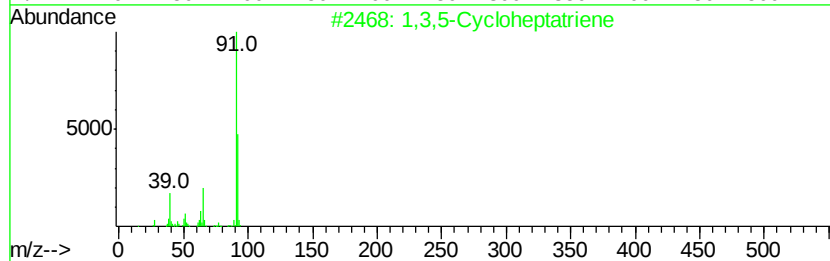
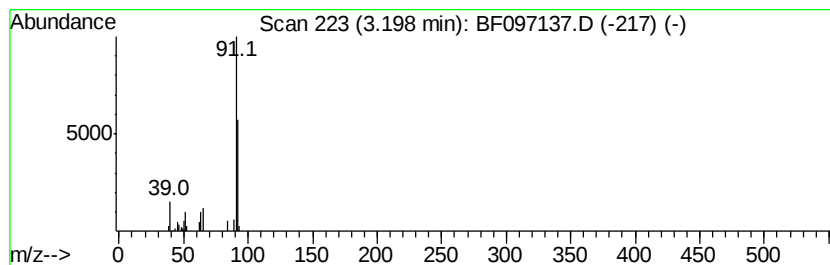
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	2.08 ng	64908	1,4-Dichlorobenzene-d4	6.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	87
2			Toluene	92	C7H8	000108-88-3	86
3			Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	78
4			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	64
5			1,5-Heptadien-3-yne	92	C7H8	003511-27-1	64



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Instrument :
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ClientSampled :
AU-06-072417-B

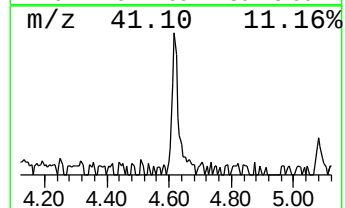
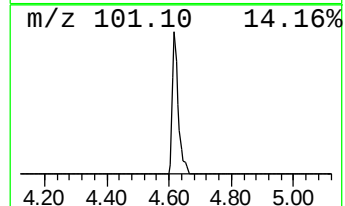
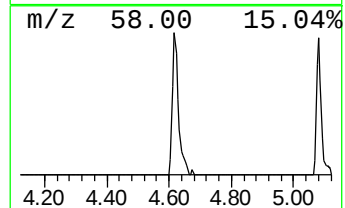
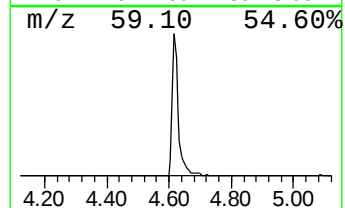
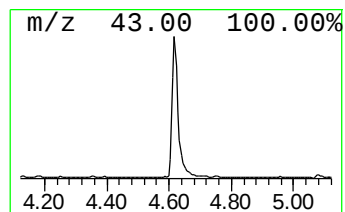
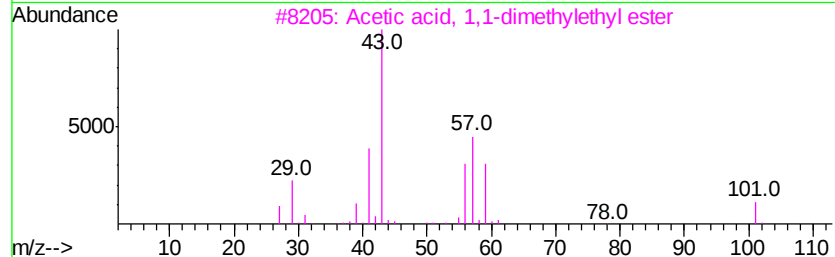
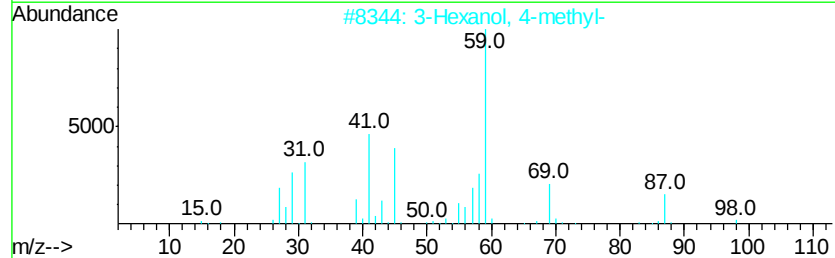
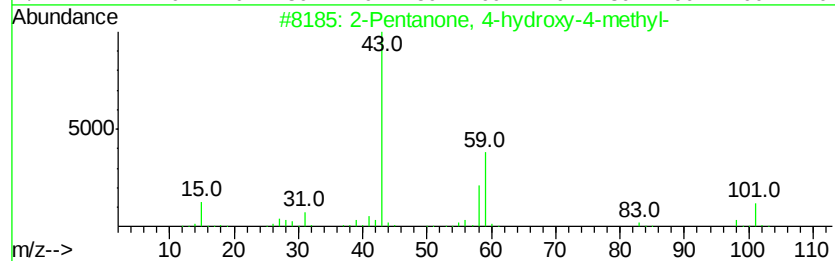
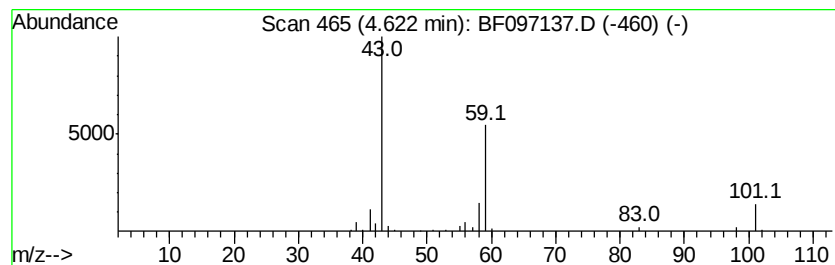
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	5.17 ng	160916	1,4-Dichlorobenzene-d4	6.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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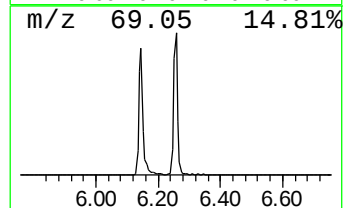
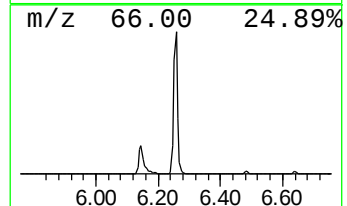
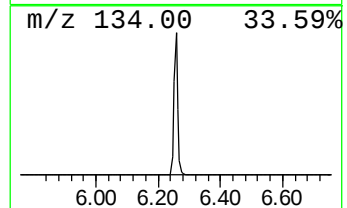
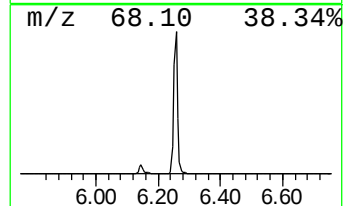
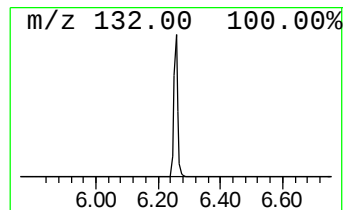
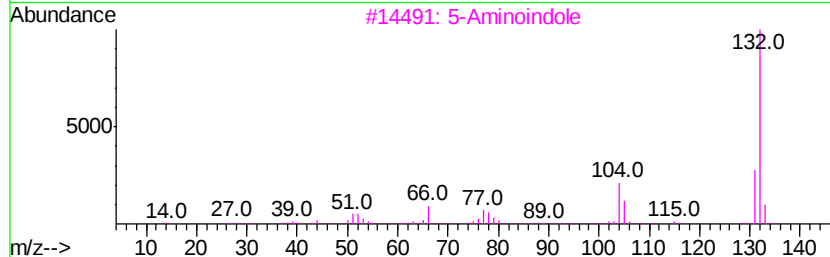
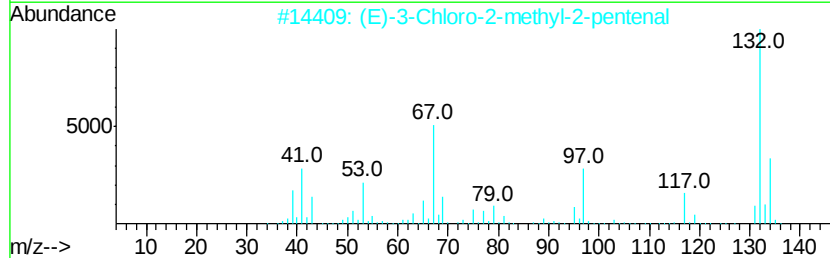
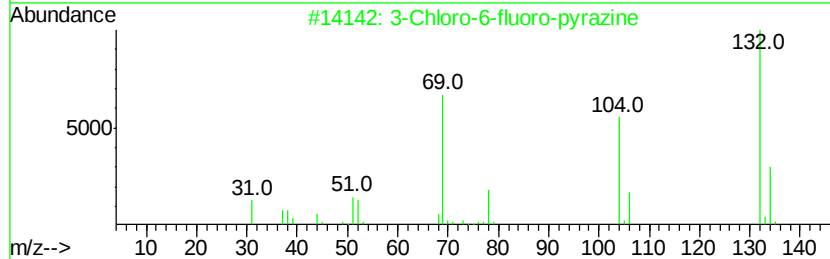
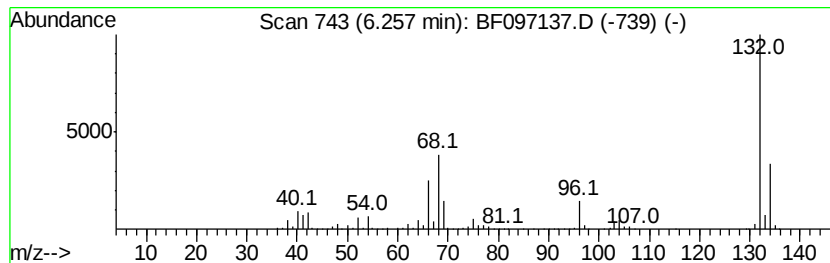
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.26 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	34.25 ng	1066740	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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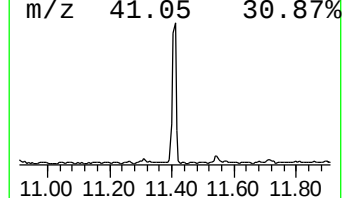
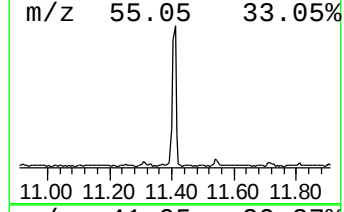
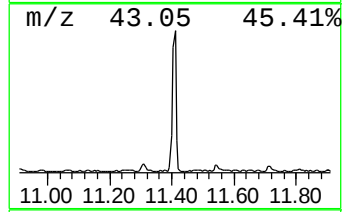
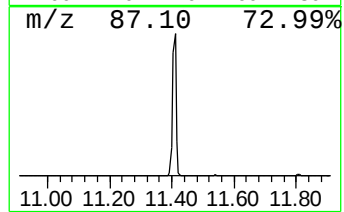
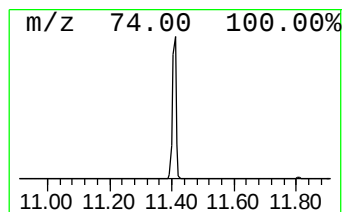
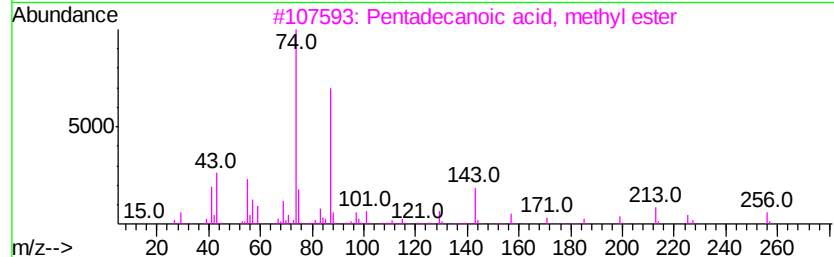
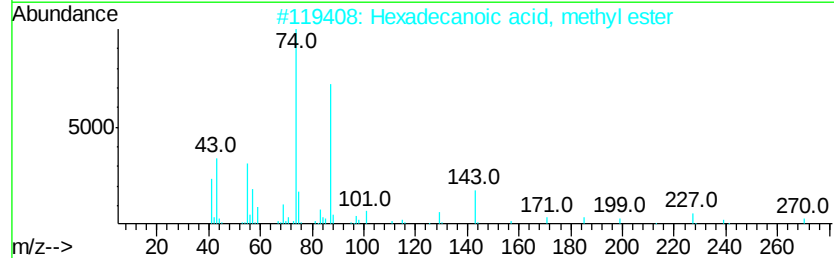
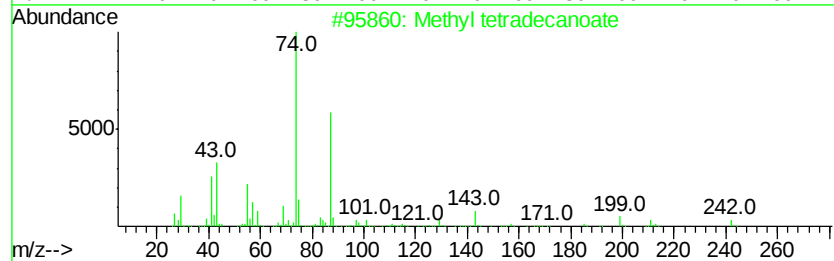
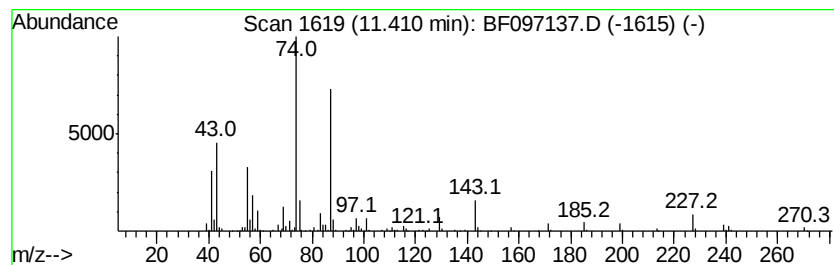
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Methyl tetradecanoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.41	19.35 ng	632237	Phenanthrene-d10	10.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
2		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90
5		Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87



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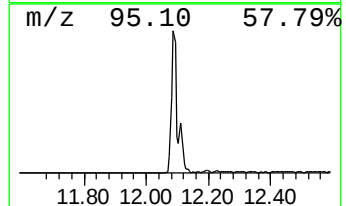
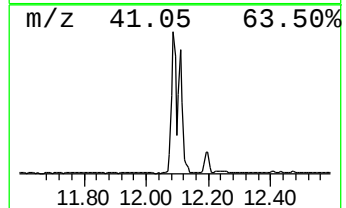
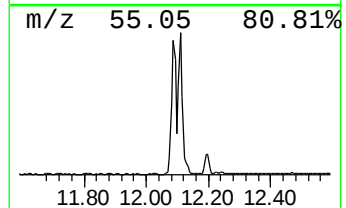
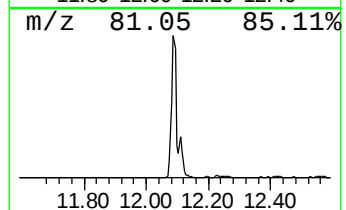
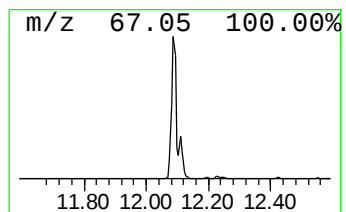
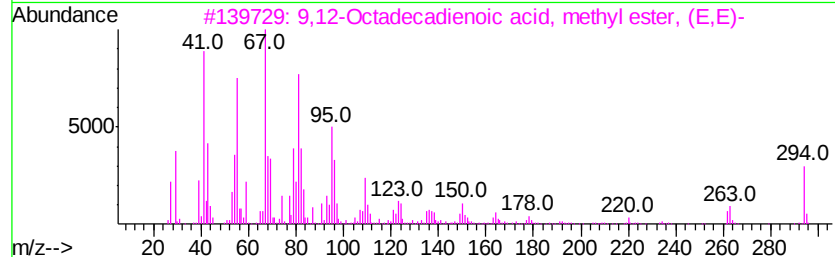
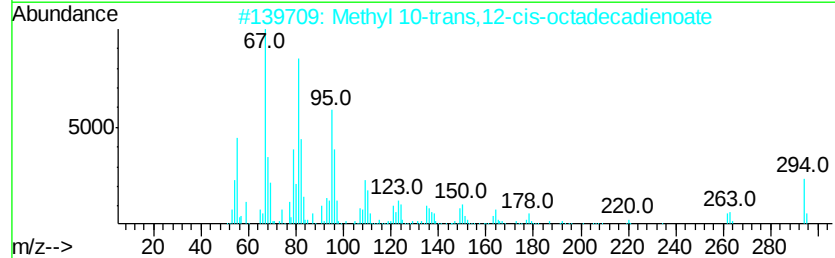
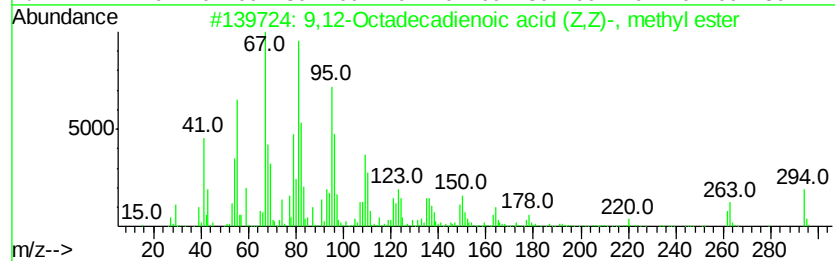
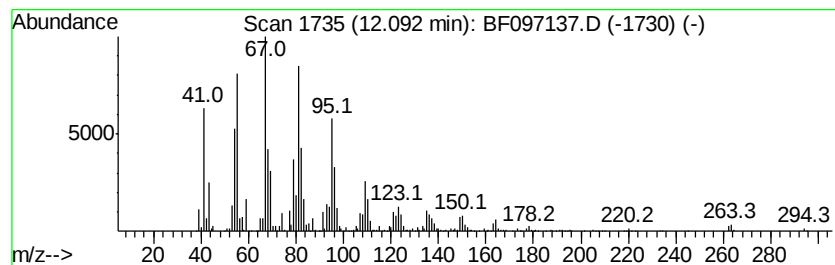
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.09	69.67 ng	2276230	Phenanthrene-d10	10.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2		Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
3		9,12-Octadecadienoic acid, methv...	294	C19H34O2	002566-97-4	98
4		8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	97
5		9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	94



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
Data File : BF097137.D
Acq On : 27 Jul 2017 22:05
Operator : SJ/JU
Sample : I4424-04 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-06-072417-B

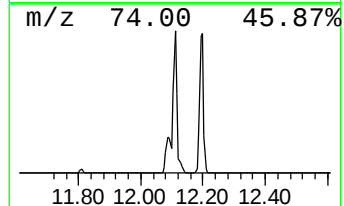
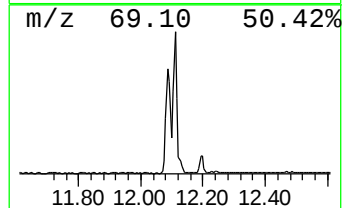
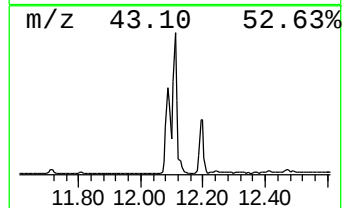
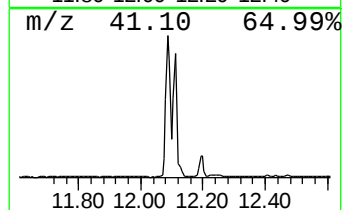
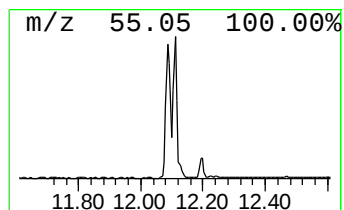
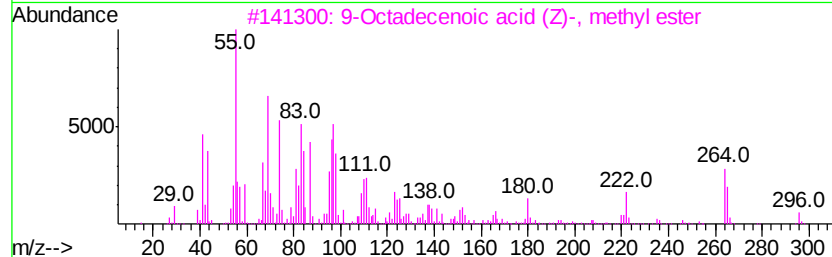
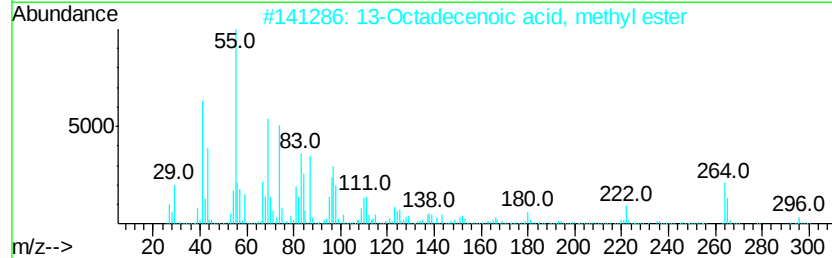
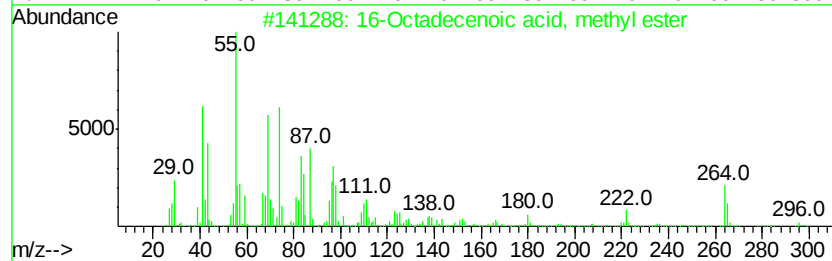
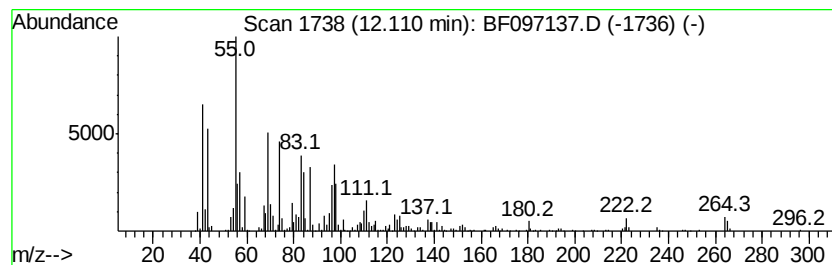
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 16-Octadecenoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.11	50.74 ng	1657860	Phenanthrene-d10	10.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	94
2		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	94
3		9-Octadecenoic acid (Z)-, methyl ester	296	C19H36O2	000112-62-9	91
4		9-Octadecenoic acid, methyl ester	296	C19H36O2	001937-62-8	91
5		11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072717\
Data File : BF097137.D
Acq On : 27 Jul 2017 22:05
Operator : SJ/JU
Sample : I4424-04 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-06-072417-B

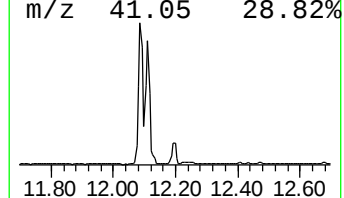
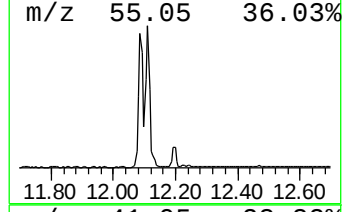
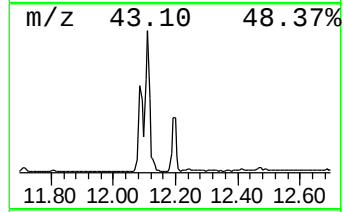
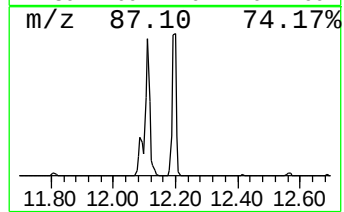
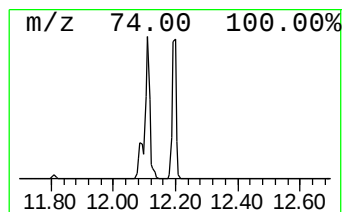
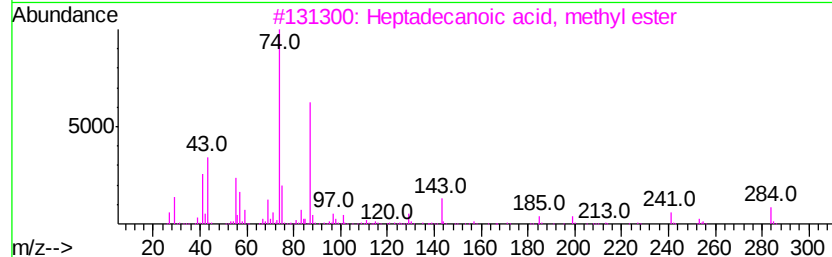
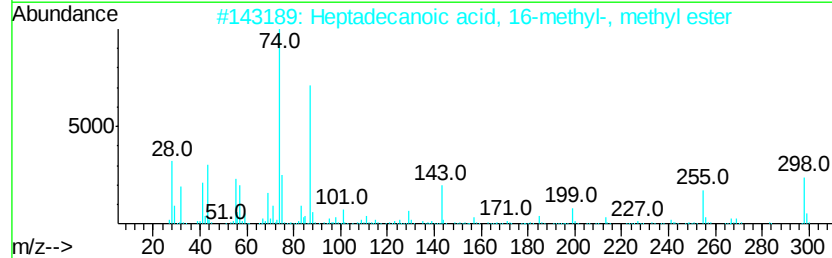
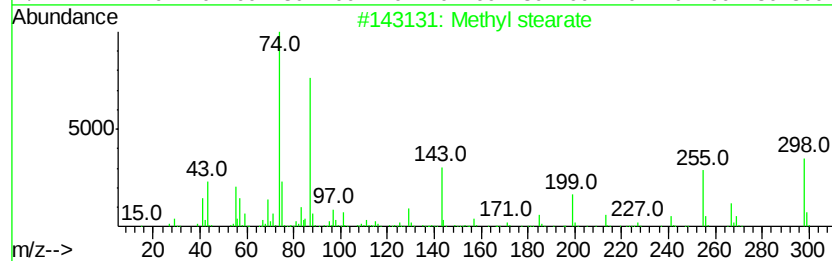
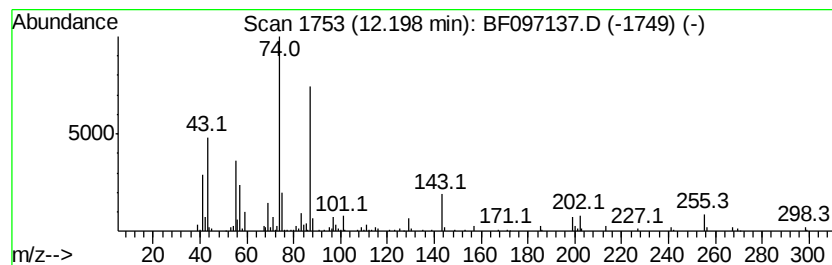
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.20	11.41 ng	372785	Phenanthrene-d10	10.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl stearate	298	C19H38O2	000112-61-8	98
2		Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
3		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
4		Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	91
5		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90



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Sample : I4424-04 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
AU-06-072417-B

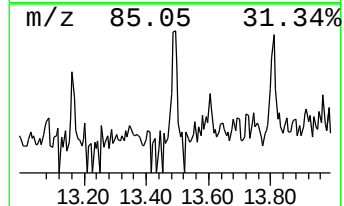
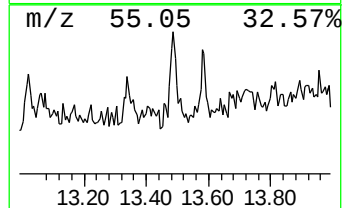
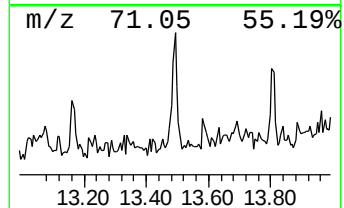
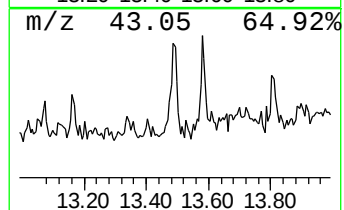
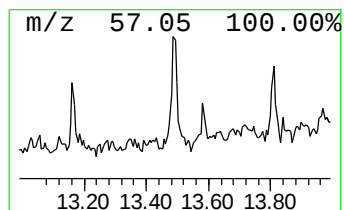
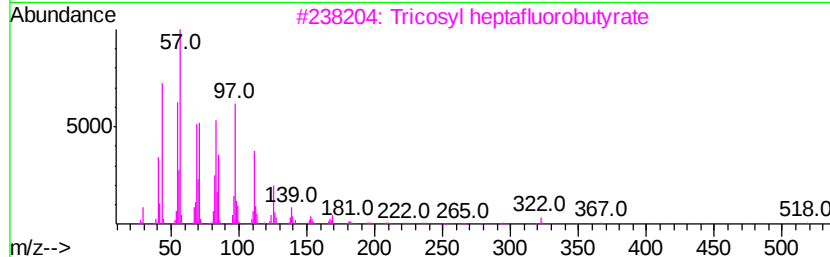
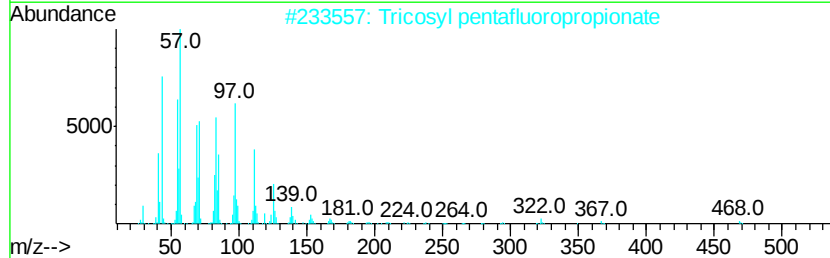
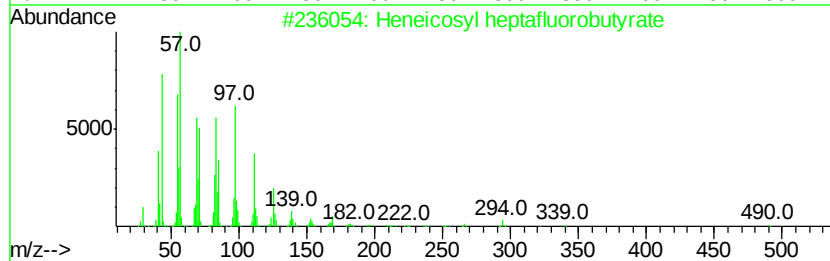
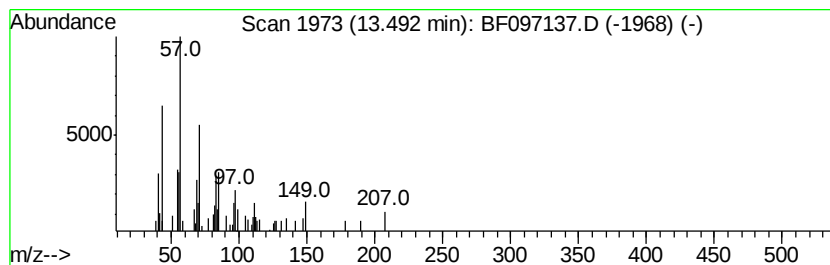
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosyl heptafluorobutyrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.13 ng	55185	Chrysene-d12	13.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosyl heptafluorobutvrate	508	C25H43F7O2	1000351-83-8	72
2		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	72
3		Tricosyl heptafluorobutvrate	536	C27H47F7O2	1000351-83-4	72
4		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	64
5		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	64



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Sample : I4424-04 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-06-072417-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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
1,3,5-Cycloheptat...	3.20	2.1	ng	64908	1	6.49	623005	20.0
2-Pentanone, 4-hy...	4.62	5.2	ng	160916	1	6.49	623005	20.0
unknown6.26	6.26	34.3	ng	1066740	1	6.49	623005	20.0
Methyl tetradecan...	11.41	19.4	ng	632237	4	10.99	653472	20.0
9,12-Octadecadien...	12.09	69.7	ng	2276230	4	10.99	653472	20.0
16-Octadecenoic a...	12.11	50.7	ng	1657860	4	10.99	653472	20.0
Methyl stearate	12.20	11.4	ng	372785	4	10.99	653472	20.0
Heneicosyl heptaf...	13.49	2.1	ng	55185	5	13.61	519240	20.0