

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092917\
 Data File : BF098938.D
 Acq On : 29 Sep 2017 9:50
 Operator : SJ/JU
 Sample : I5472-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1-2-3-4-COMP

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-BF092317.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	2.240	22	26	40	rVB	137444	208845	5.47%	0.579%
2	5.151	516	521	531	rVB	587592	786129	20.58%	2.181%
3	5.545	582	588	591	rBV	3267182	3364055	88.08%	9.331%
4	6.545	752	758	761	rBV	3091699	3424181	89.66%	9.498%
5	6.686	777	782	785	rBV	3415486	3490126	91.38%	9.681%
6	6.739	788	791	798	rVB	51178	42786	1.12%	0.119%
7	6.916	817	821	824	rBV	1032595	814646	21.33%	2.260%
8	7.075	843	848	851	rBV	2929360	2653883	69.49%	7.361%
9	7.481	911	917	920	rBV	1991702	2184016	57.19%	6.058%
10	8.198	1034	1039	1042	rBV	1276601	1101959	28.85%	3.057%
11	9.274	1216	1222	1225	rBV	3764231	3819178	100.00%	10.594%
12	9.663	1283	1288	1291	rBV	642178	535427	14.02%	1.485%
13	9.874	1319	1324	1328	rBV2	36284	38586	1.01%	0.107%
14	9.951	1332	1337	1341	rBV	1304429	1224994	32.07%	3.398%
15	10.139	1365	1369	1376	rVB5	43535	74136	1.94%	0.206%
16	10.351	1402	1405	1406	rBV	56241	49536	1.30%	0.137%
17	10.369	1406	1408	1411	rVB2	78179	81621	2.14%	0.226%
18	10.586	1441	1445	1449	rBV2	37101	47406	1.24%	0.131%
19	10.745	1464	1472	1475	rBV	2269027	2244405	58.77%	6.226%
20	10.845	1486	1489	1500	rBV	96373	110966	2.91%	0.308%
21	11.086	1526	1530	1535	rVB6	32015	53215	1.39%	0.148%
22	11.439	1586	1590	1593	rBV	1376354	1218723	31.91%	3.381%
23	11.957	1672	1678	1685	rBV2	254216	355398	9.31%	0.986%
24	12.133	1705	1708	1716	rVB10	20646	41790	1.09%	0.116%
25	12.739	1807	1811	1816	rBV	112002	122502	3.21%	0.340%
26	13.027	1855	1860	1863	rBV2	3418877	3496948	91.56%	9.700%
27	13.139	1871	1879	1888	rBV	1021421	1890286	49.49%	5.243%
28	13.368	1912	1918	1927	rVB	217952	413577	10.83%	1.147%
29	13.904	2006	2009	2013	rVB	197020	189519	4.96%	0.526%
30	14.080	2035	2039	2042	rBV	1041517	877883	22.99%	2.435%
31	14.433	2094	2099	2105	rVB2	47562	82538	2.16%	0.229%
32	14.539	2113	2117	2123	rVB6	28469	42769	1.12%	0.119%
33	14.921	2179	2182	2190	rVB3	62192	93271	2.44%	0.259%
34	15.309	2243	2248	2255	rBV10	45458	84058	2.20%	0.233%

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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 >
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35	15.574	2288	2293	2304	rVB	526870	688783	18.03%	1.911%
36	16.027	2367	2370	2376	rVB3	29726	41948	1.10%	0.116%
37	16.603	2464	2468	2475	rVB9	29206	60805	1.59%	0.169%

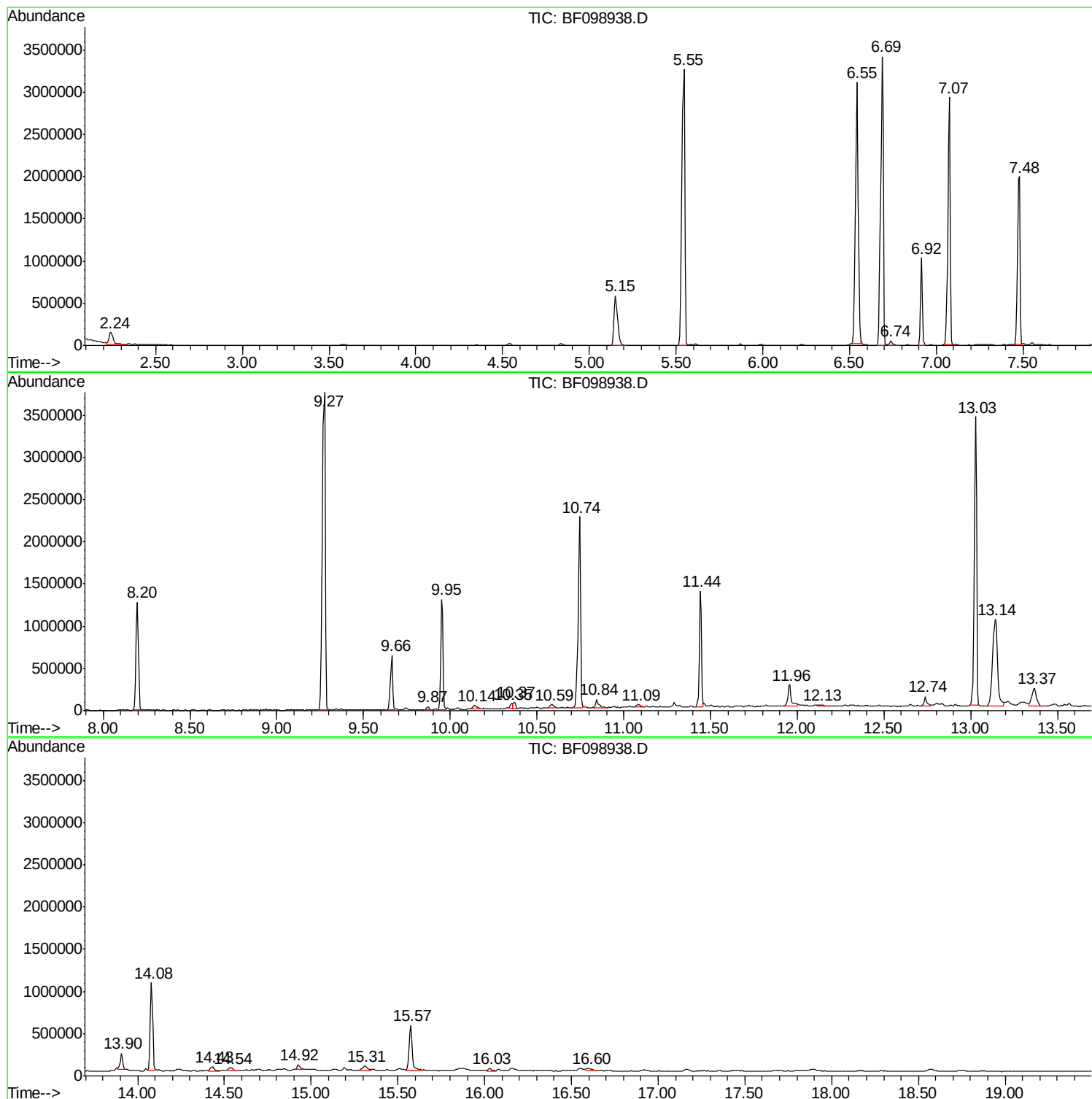
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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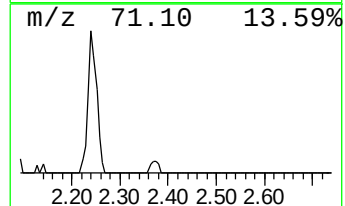
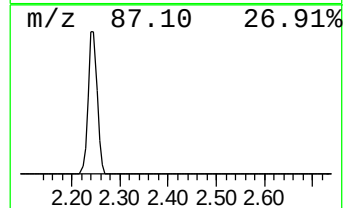
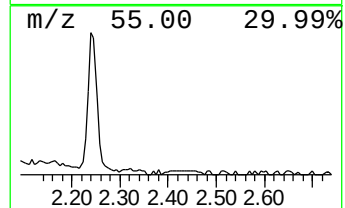
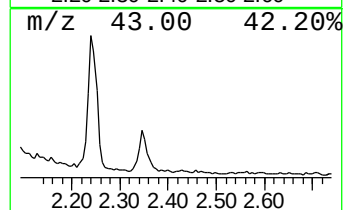
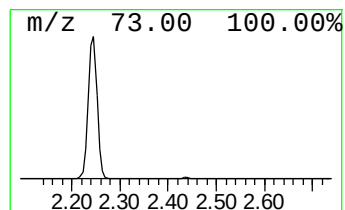
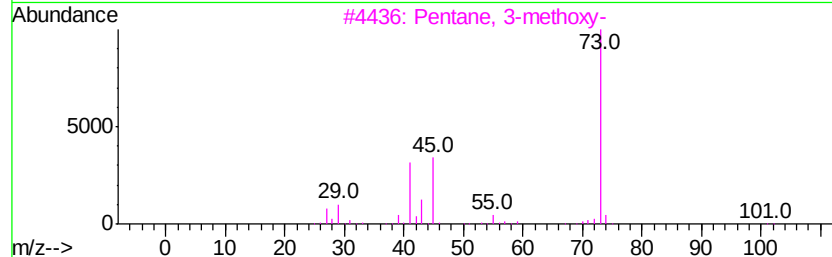
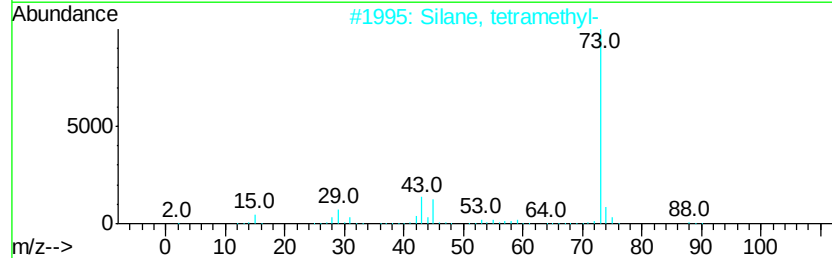
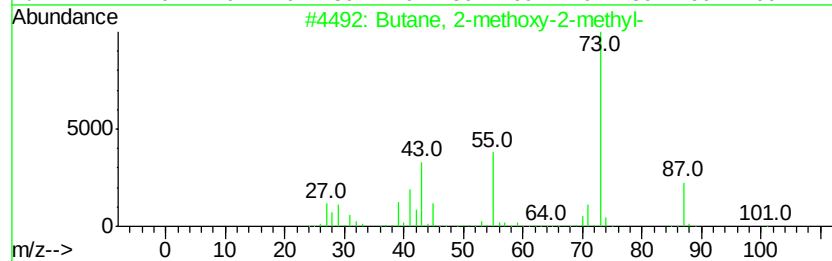
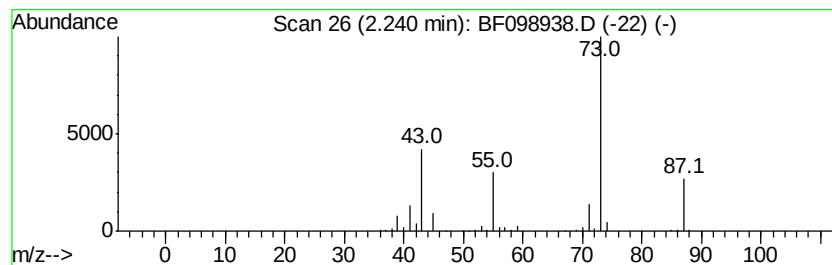
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	5.13 ng	208845	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	27
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		1,4-Butanediamine	88	C4H12N2	000110-60-1	10
5		1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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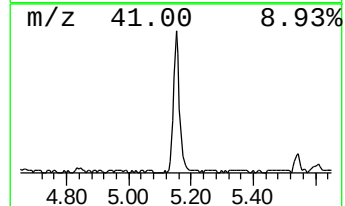
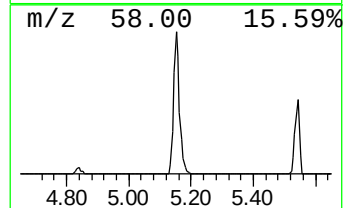
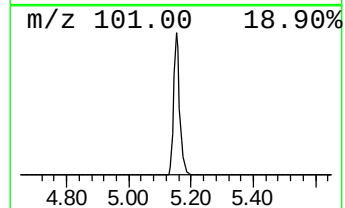
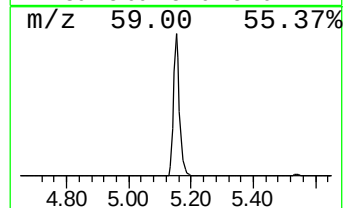
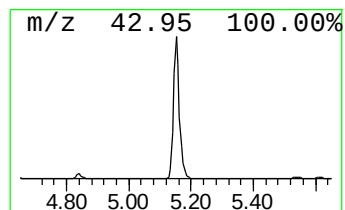
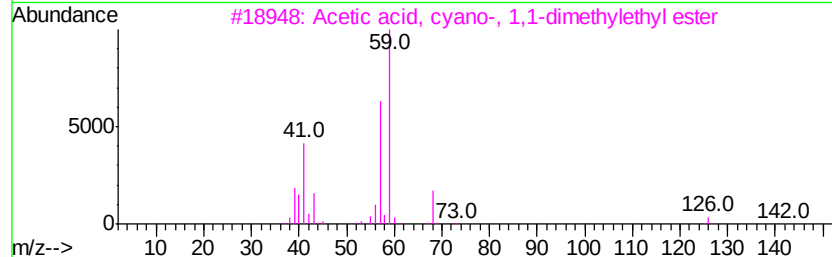
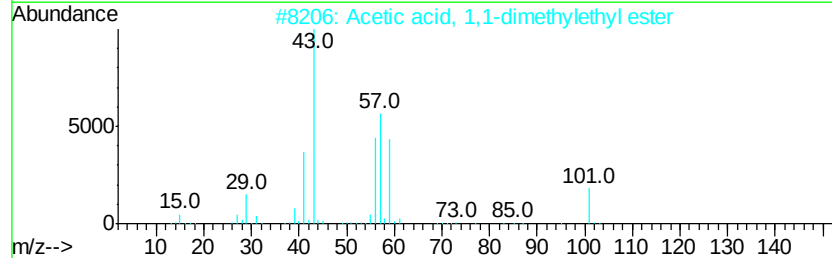
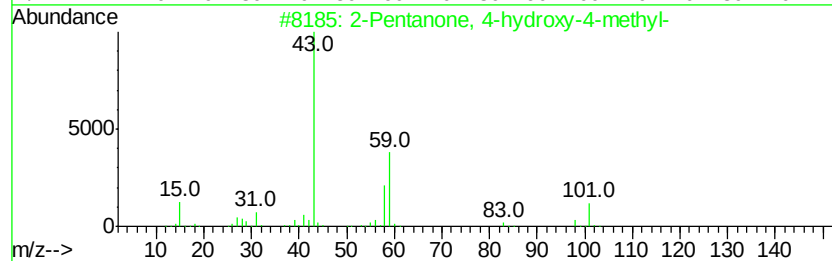
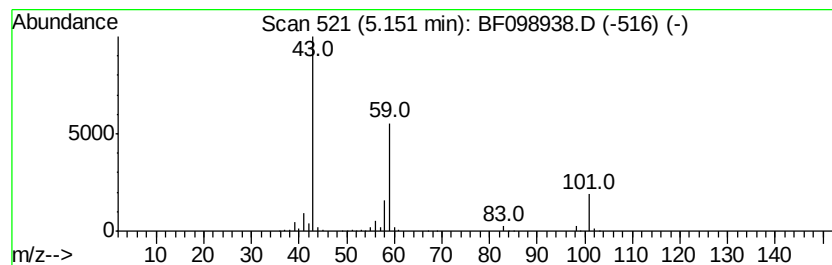
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	19.30 ng	786129	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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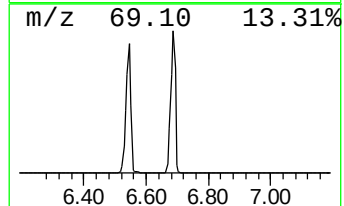
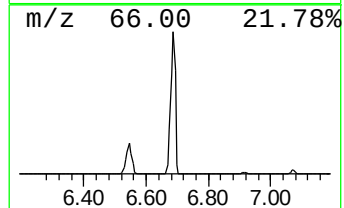
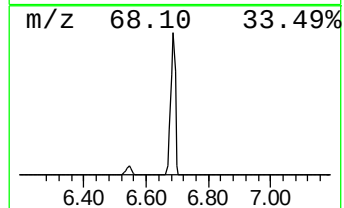
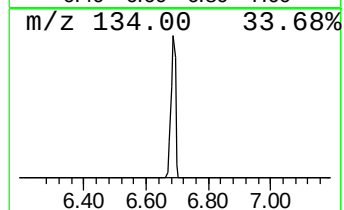
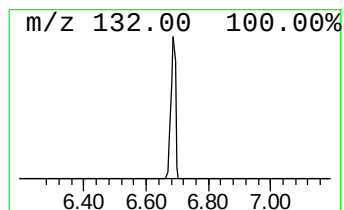
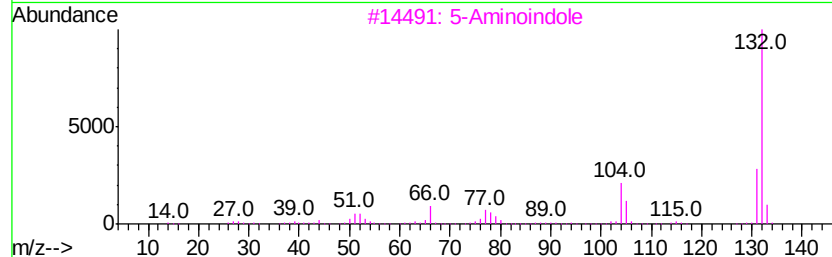
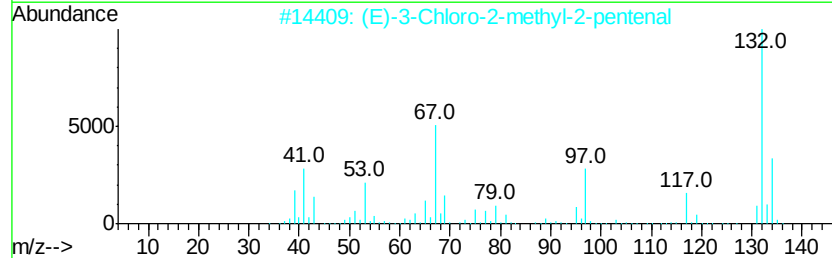
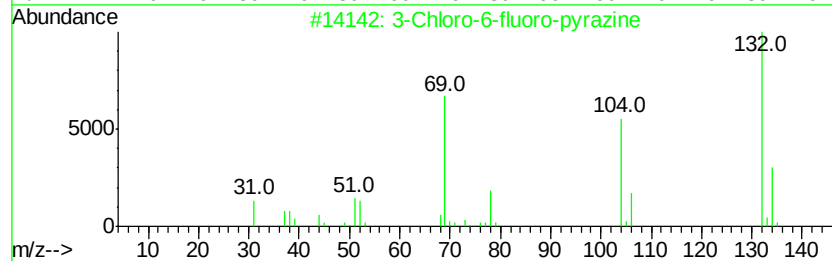
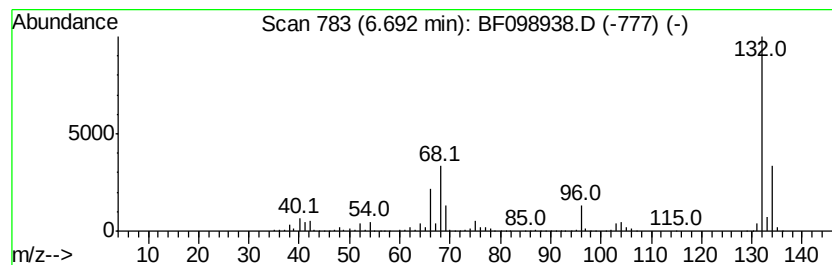
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	85.68 ng	3490130	1,4-Dichlorobenzene-d4	6.92

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		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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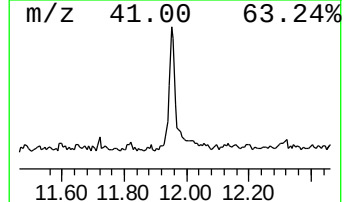
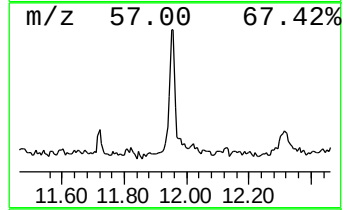
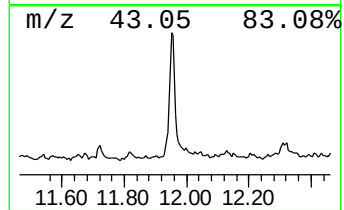
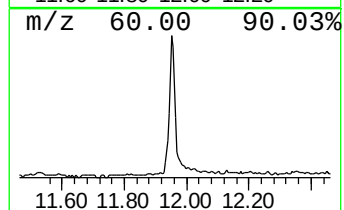
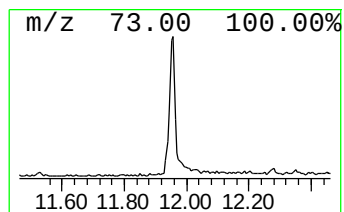
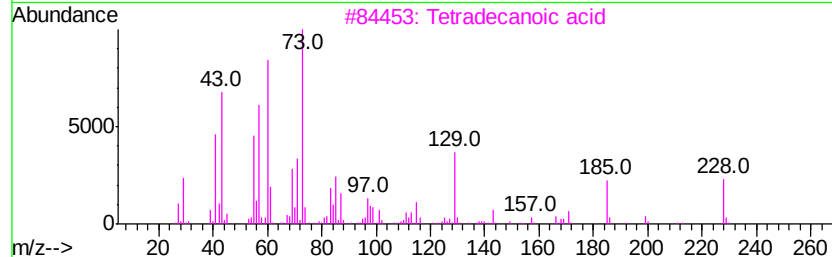
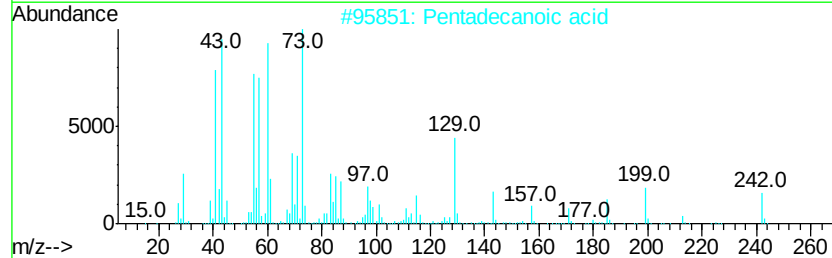
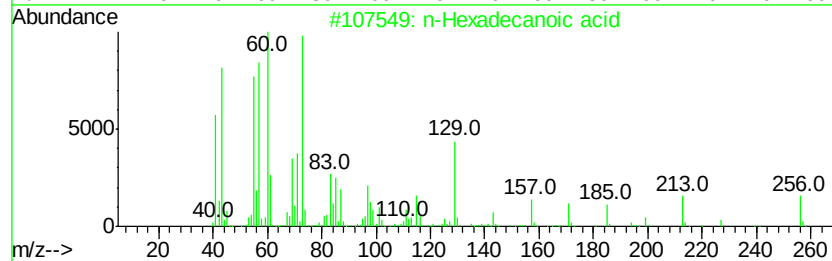
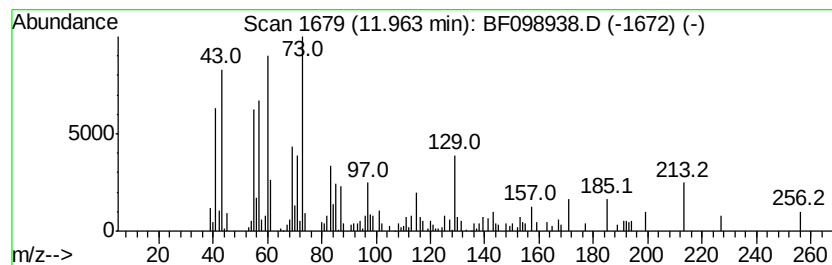
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	5.83 ng	355398	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		Tridecanoic acid	214	C13H26O2	000638-53-9	81
5		Undecanoic acid	186	C11H22O2	000112-37-8	80



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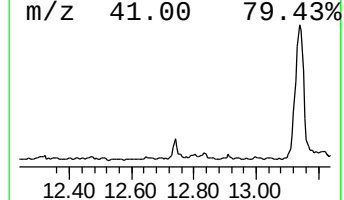
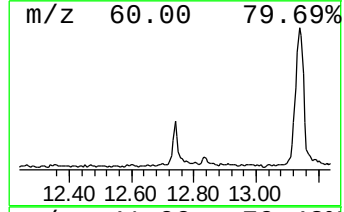
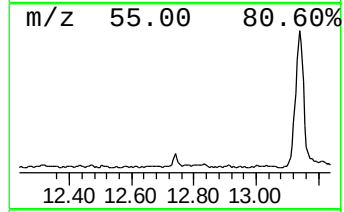
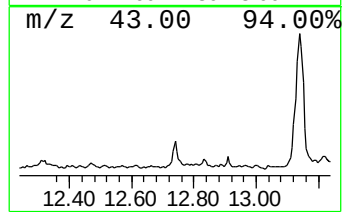
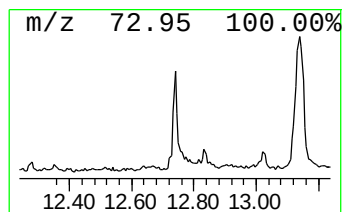
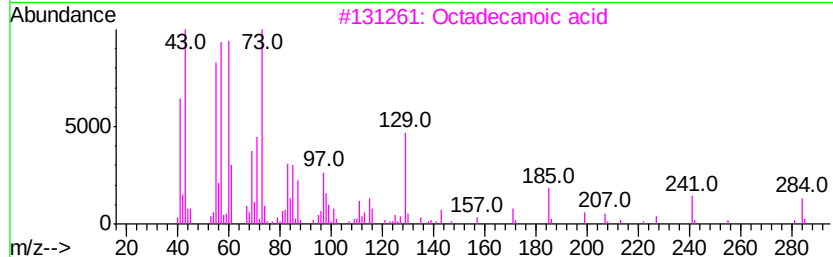
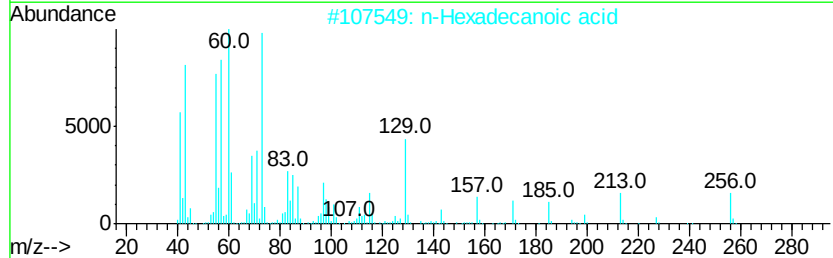
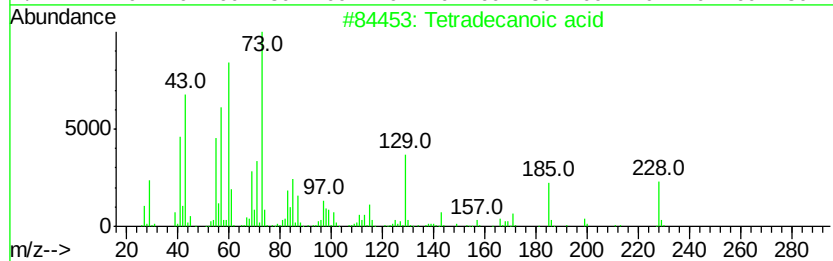
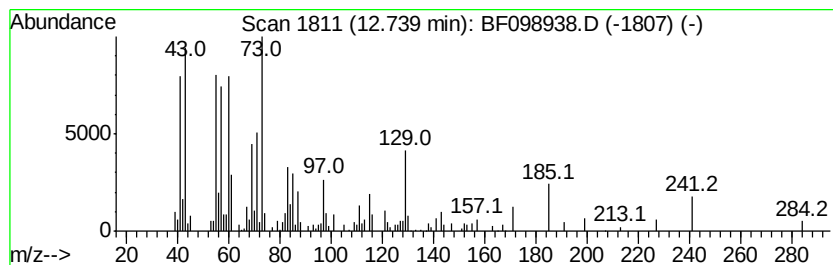
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Tetradecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.01 ng	122502	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3		Octadecanoic acid	284	C18H36O2	000057-11-4	43
4		Tridecanoic acid	214	C13H26O2	000638-53-9	43
5		L-Homoserine lactone, N,N-dimethyl-	129	C6H11NO2	1000374-45-7	25



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Data File : BF098938.D
Acq On : 29 Sep 2017 9:50
Operator : SJ/JU
Sample : I5472-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-3-4-COMP

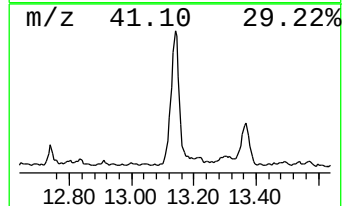
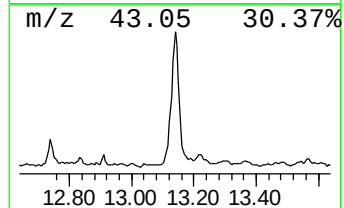
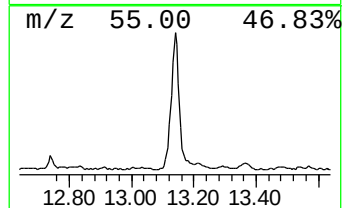
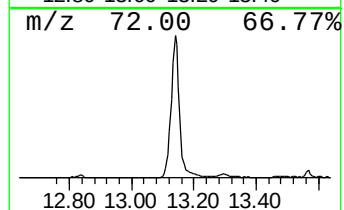
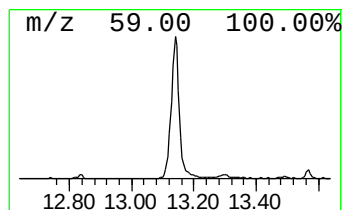
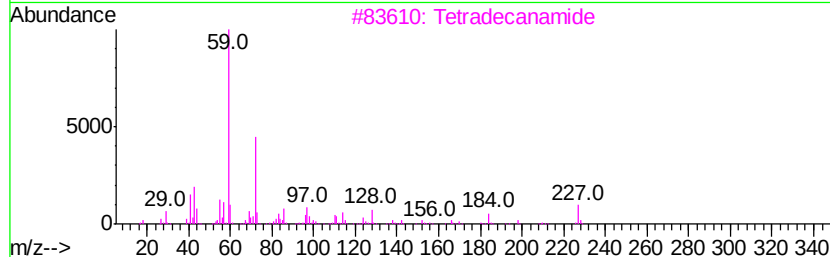
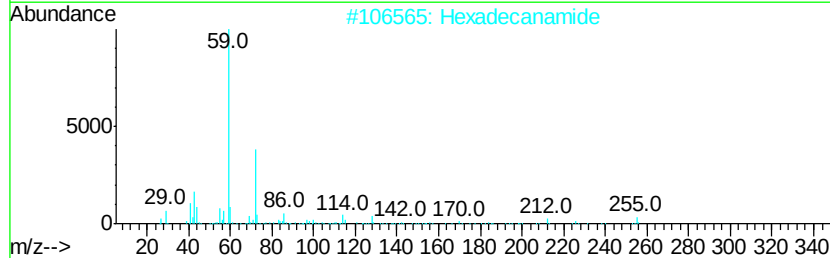
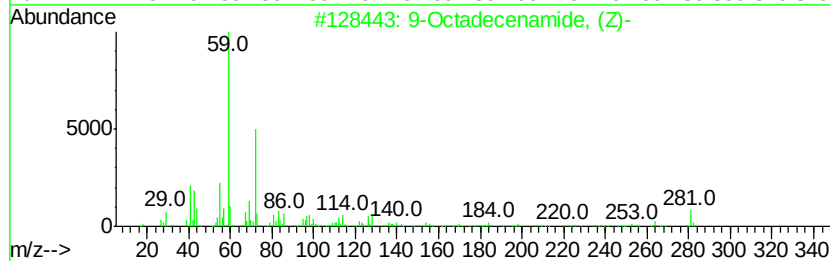
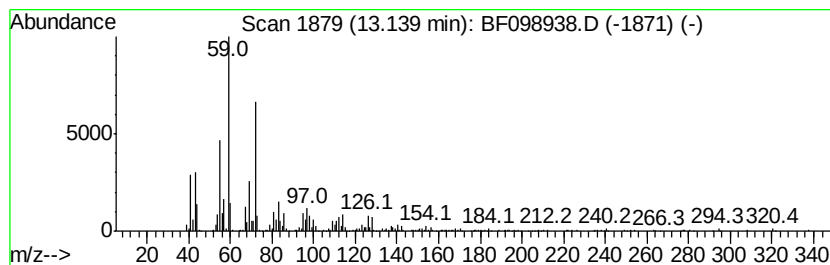
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	43.06 ng	1890290	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Hexadecanamide	255	C16H33NO	000629-54-9	78
3		Tetradecanamide	227	C14H29NO	000638-58-4	64
4		Decanamide-	171	C10H21NO	002319-29-1	59
5		2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	46



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092917\
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Acq On : 29 Sep 2017 9:50
Operator : SJ/JU
Sample : I5472-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-3-4-COMP

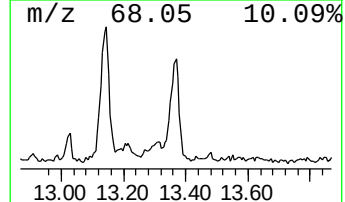
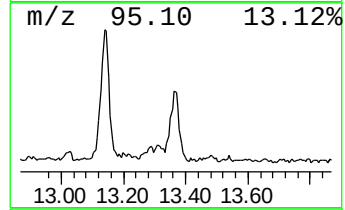
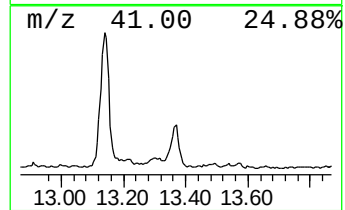
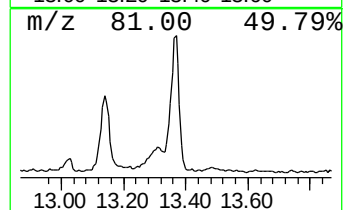
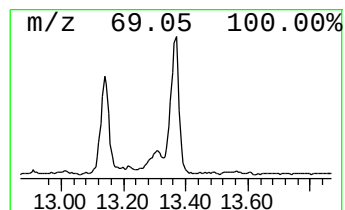
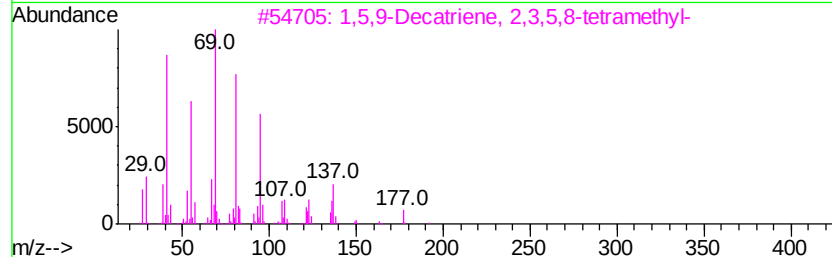
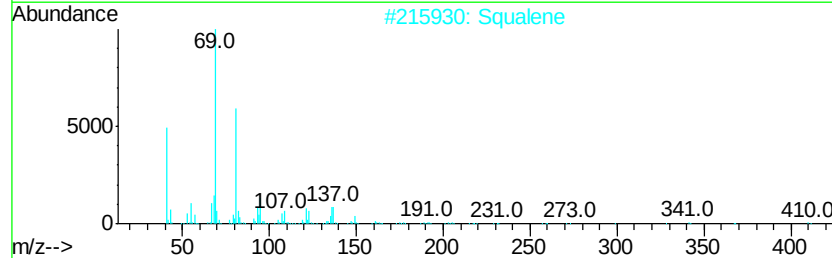
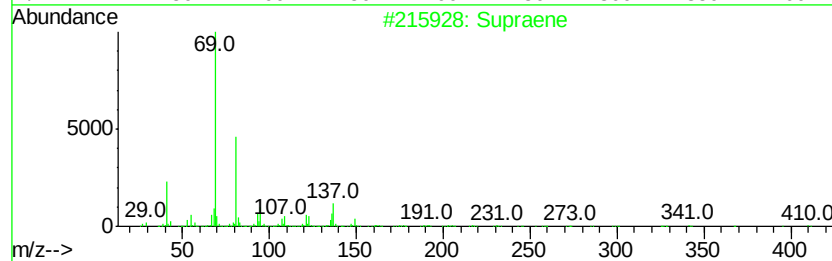
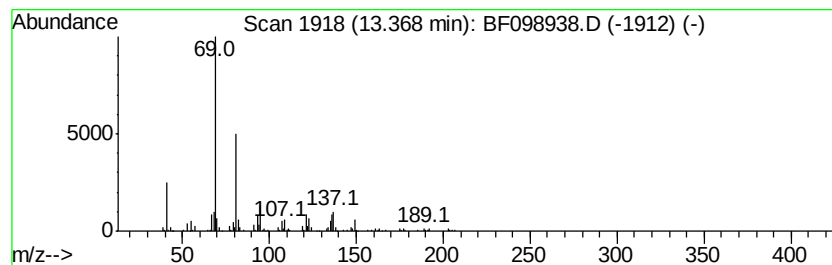
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	9.42 ng	413577	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	80
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092917\
Data File : BF098938.D
Acq On : 29 Sep 2017 9:50
Operator : SJ/JU
Sample : I5472-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

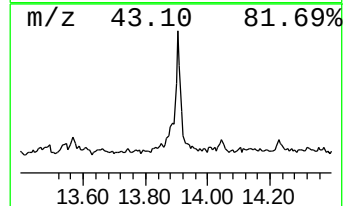
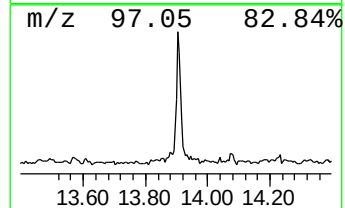
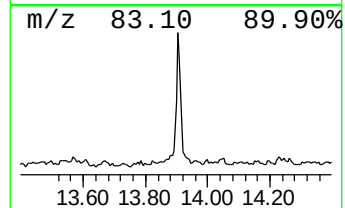
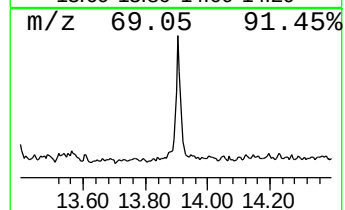
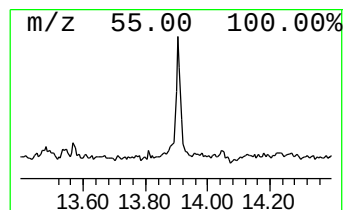
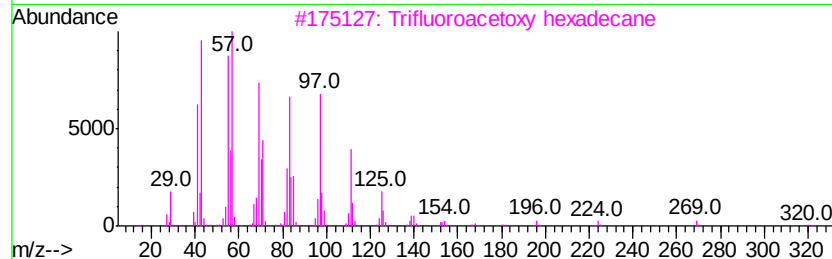
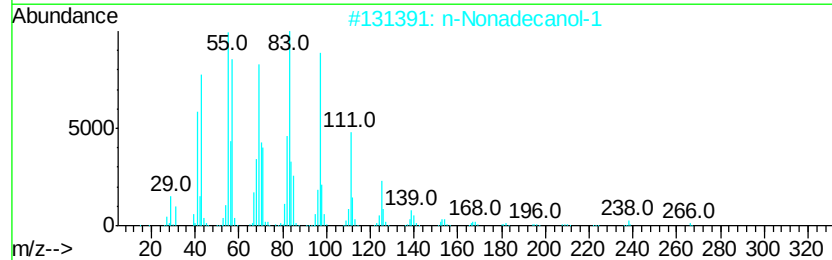
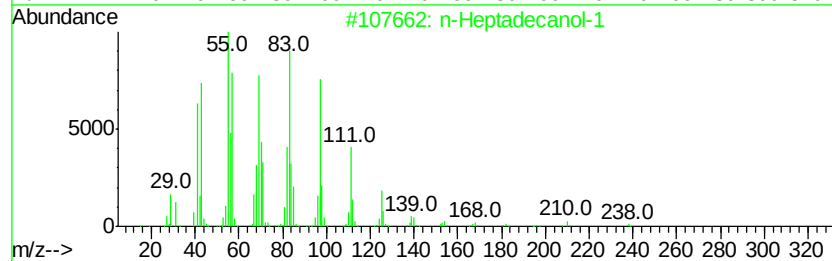
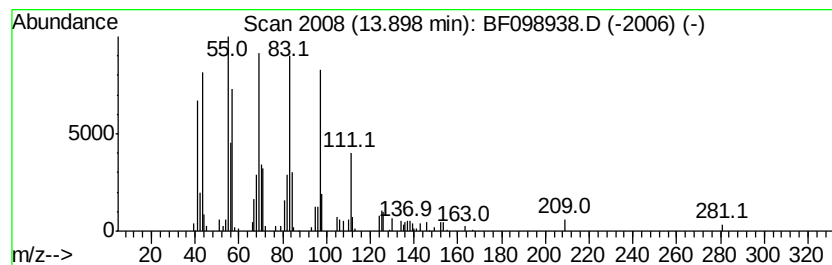
Instrument :
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ClientSampleId :
TP-1-2-3-4-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Heptadecanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	4.32 ng	189519	Chrysene-d12	14.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	n-Pentadecanol	228	C15H32O	000629-76-5	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092917\
Data File : BF098938.D
Acq On : 29 Sep 2017 9:50
Operator : SJ/JU
Sample : I5472-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

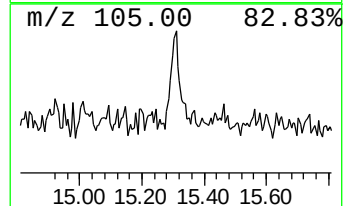
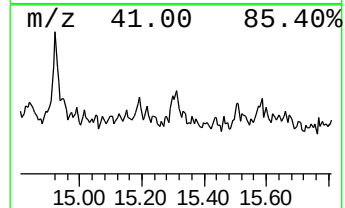
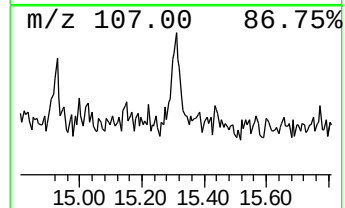
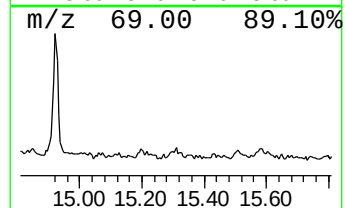
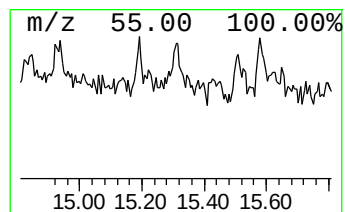
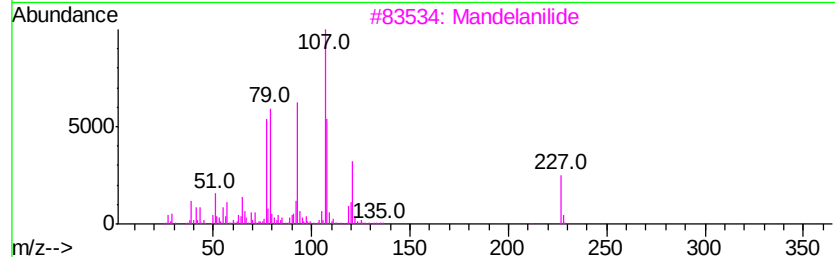
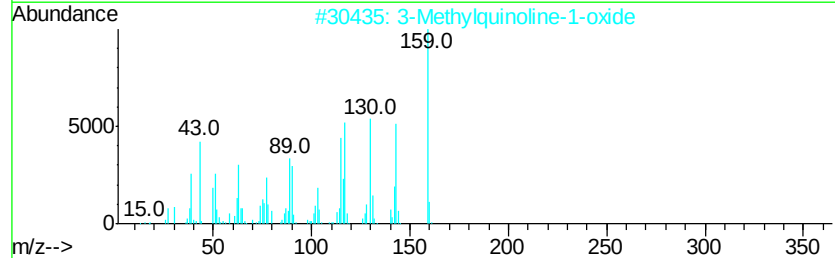
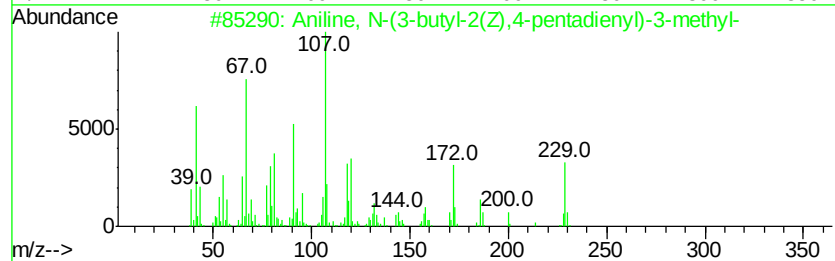
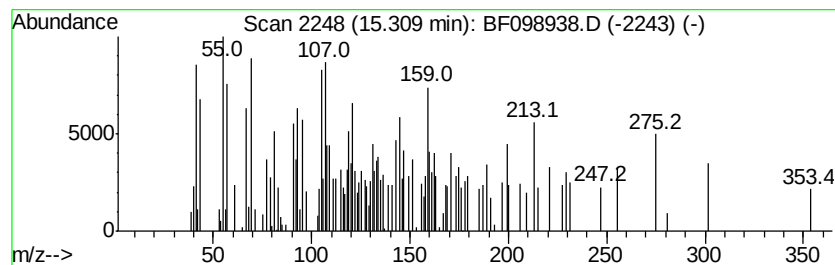
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.31 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.31	2.44 ng	84058	Perylene-d12	15.57		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aniline, N-(3-butyl-2(Z),4-penta...	229	C16H23N	1000142-27-8	11	
2	3-Methylquinoline-1-oxide	159	C10H9NO	001873-55-8	11	
3	Mandelanilide	227	C14H13NO2	004410-33-7	10	
4	Cyclohexaneacetamide, N-(2-methy...	231	C15H21NO	1000317-30-8	10	
5	Ethanone, 2-(1-methylethoxy)-1,2...	254	C17H18O2	006652-28-4	10	



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Operator : SJ/JU
Sample : I5472-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-3-4-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.24	5.1 ng		208845	1	6.92	814646	20.0
2-Pentanone, 4-hy...	5.15	19.3 ng		786129	1	6.92	814646	20.0
unknown6.69	6.69	85.7 ng		3490130	1	6.92	814646	20.0
n-Hexadecanoic acid	11.96	5.8 ng		355398	4	11.44	1218720	20.0
Tetradecanoic acid	12.74	2.0 ng		122502	4	11.44	1218720	20.0
9-Octadecenamide,...	13.14	43.1 ng		1890290	5	14.08	877883	20.0
Supraene	13.37	9.4 ng		413577	5	14.08	877883	20.0
n-Heptadecanol-1	13.90	4.3 ng		189519	5	14.08	877883	20.0
unknown15.31	15.31	2.4 ng		84058	6	15.57	688783	20.0