

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
 Data File : BF096284.D
 Acq On : 29 Jun 2017 11:46
 Operator : SJ/MA
 Sample : I3899-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11940

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-BF062717.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	4.969	485	490	497	rVB	605053	752056	21.54%	2.300%
2	5.387	556	561	564	rBV	3588803	3444169	98.63%	10.533%
3	6.398	728	733	736	rBV	3549669	3415123	97.79%	10.444%
4	6.540	752	757	760	rBV	3603515	3363150	96.31%	10.285%
5	6.769	792	796	800	rBV	1269010	1007088	28.84%	3.080%
6	6.928	818	823	826	rBV	2812031	2518183	72.11%	7.701%
7	7.328	886	891	894	rBV	2261220	2167047	62.05%	6.627%
8	7.416	903	906	910	rVB	42719	35449	1.02%	0.108%
9	7.739	956	961	964	rBV2	35108	42698	1.22%	0.131%
10	8.051	1009	1014	1017	rBV	1571575	1360688	38.96%	4.161%
11	8.957	1163	1168	1173	rBV2	34934	40226	1.15%	0.123%
12	9.128	1192	1197	1200	rBV	3638076	3492159	100.00%	10.679%
13	9.516	1256	1263	1267	rBV	914279	815628	23.36%	2.494%
14	9.745	1300	1302	1307	rVB	37974	35556	1.02%	0.109%
15	9.804	1307	1312	1316	rBV	1512425	1369937	39.23%	4.189%
16	10.086	1354	1360	1366	rBV	74663	115103	3.30%	0.352%
17	10.245	1385	1387	1391	rVB	88262	68343	1.96%	0.209%
18	10.469	1420	1425	1427	rBV	30940	41092	1.18%	0.126%
19	10.586	1440	1445	1448	rBV	2059485	1837779	52.63%	5.620%
20	10.716	1465	1467	1470	rBV	113179	115814	3.32%	0.354%
21	11.169	1540	1544	1546	rBV2	88776	76847	2.20%	0.235%
22	11.198	1546	1549	1553	rVB	36338	35274	1.01%	0.108%
23	11.280	1559	1563	1567	rBV2	1345956	1189037	34.05%	3.636%
24	11.516	1600	1603	1607	rVB	222145	176881	5.07%	0.541%
25	11.592	1613	1616	1622	rVB	68433	58084	1.66%	0.178%
26	11.816	1650	1654	1658	rBV	128144	128485	3.68%	0.393%
27	11.998	1682	1685	1688	rVB	53085	40568	1.16%	0.124%
28	12.604	1784	1788	1796	rBV	113107	141229	4.04%	0.432%
29	12.698	1802	1804	1811	rVB2	23898	38970	1.12%	0.119%
30	12.869	1828	1833	1836	rBV	2796750	2549799	73.01%	7.798%
31	13.769	1982	1986	1991	rBV	206288	209641	6.00%	0.641%
32	13.910	2006	2010	2014	rBV	961185	884942	25.34%	2.706%
33	14.404	2091	2094	2097	rBV	40425	35074	1.00%	0.107%
34	15.027	2197	2200	2207	rVB4	31005	45270	1.30%	0.138%

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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 >
Peak separation: 5

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35	15.333	2248	2252	2256	rBV	646466	794955	22.76%	2.431%
36	15.374	2256	2259	2268	rVB4	58835	116604	3.34%	0.357%
37	15.810	2330	2333	2337	rBV2	29346	41806	1.20%	0.128%
38	15.851	2337	2340	2345	rVB5	36642	53469	1.53%	0.164%
39	16.027	2368	2370	2377	rVB7	29554	45913	1.31%	0.140%

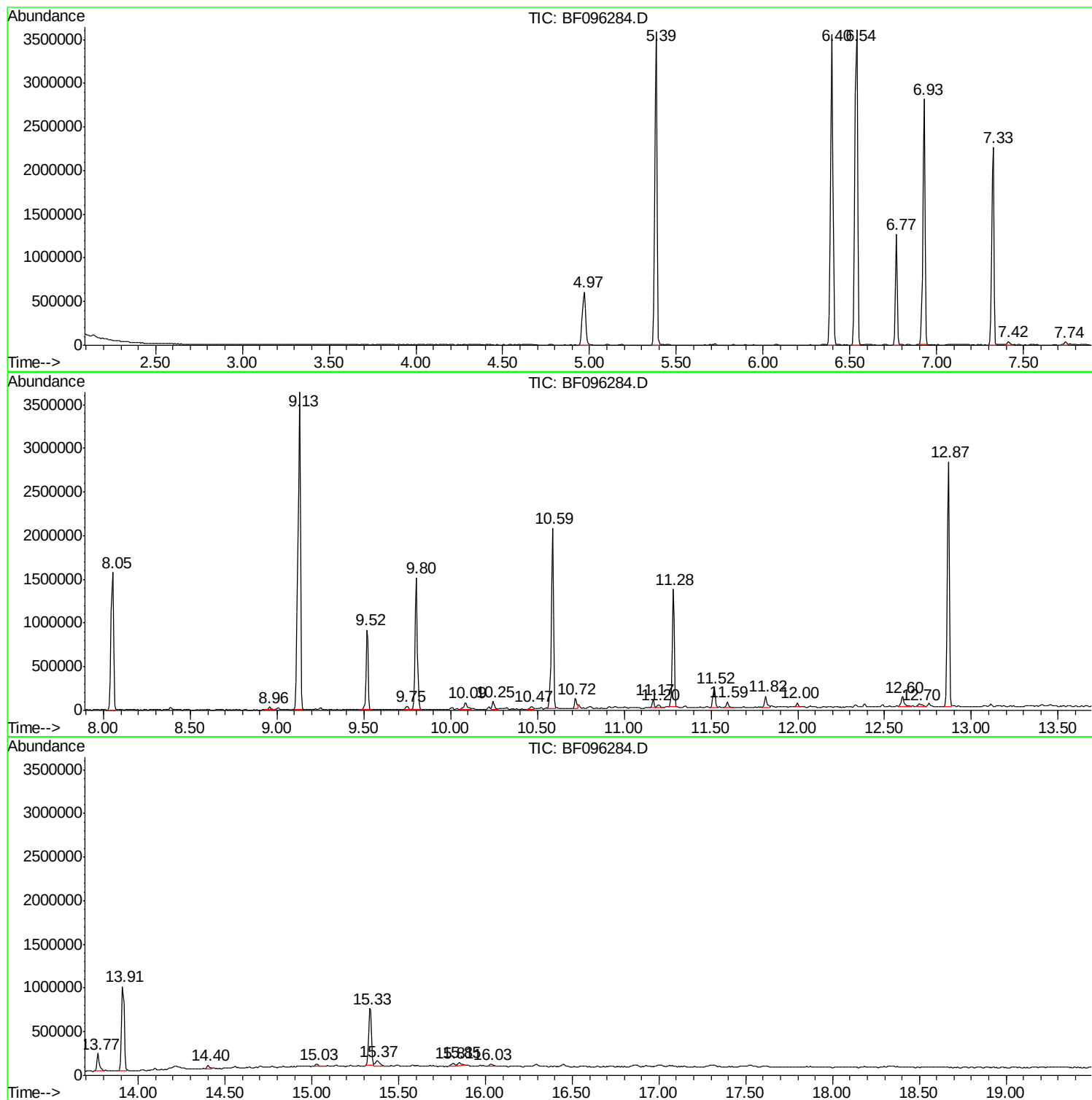
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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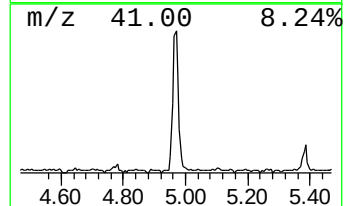
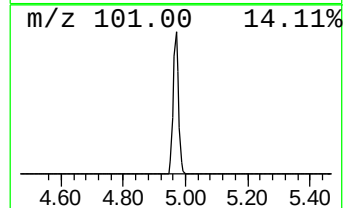
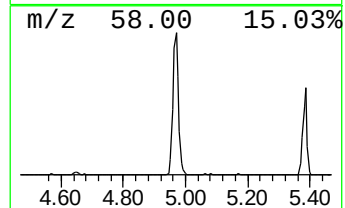
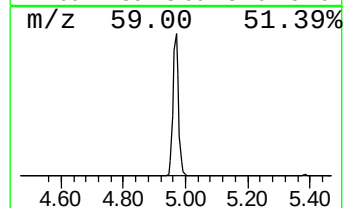
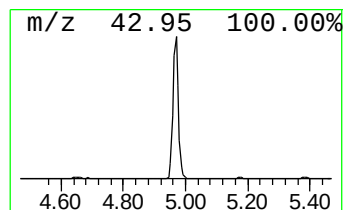
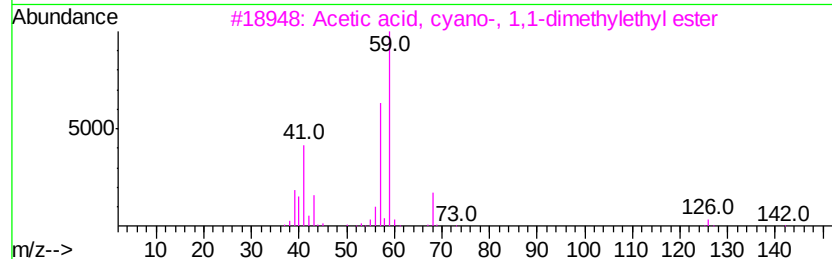
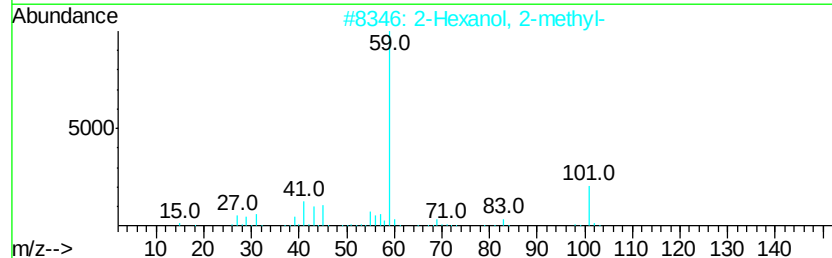
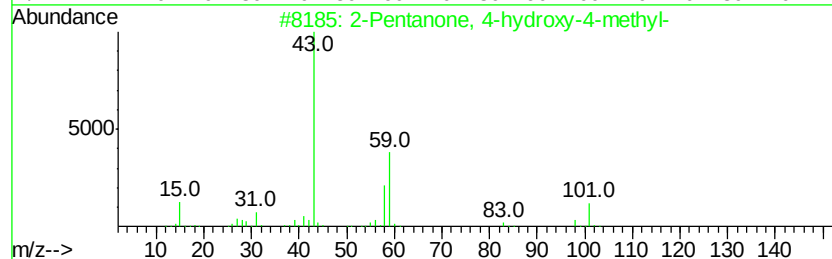
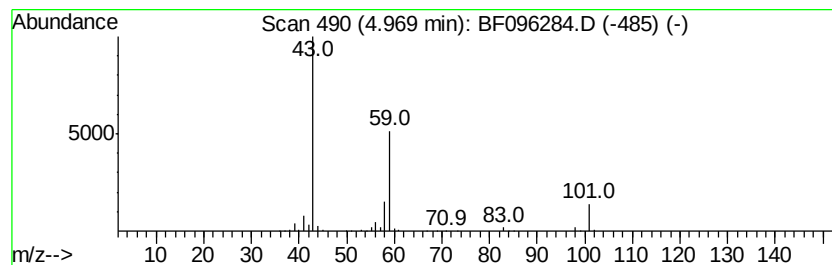
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown4.97 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	14.94 ng	752056	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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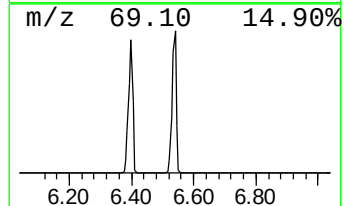
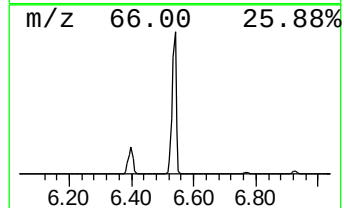
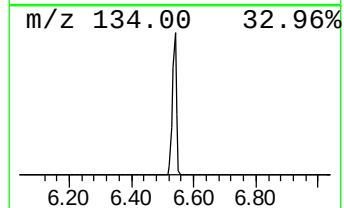
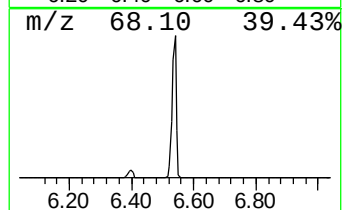
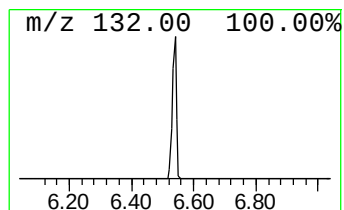
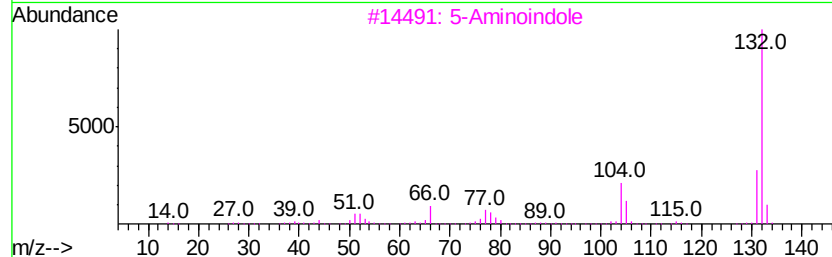
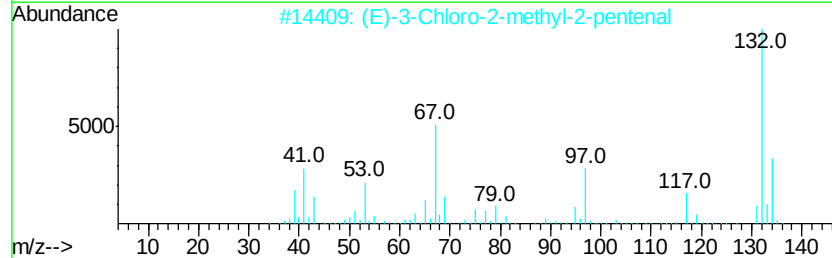
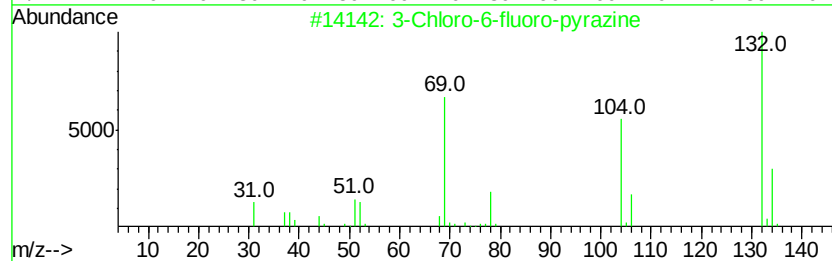
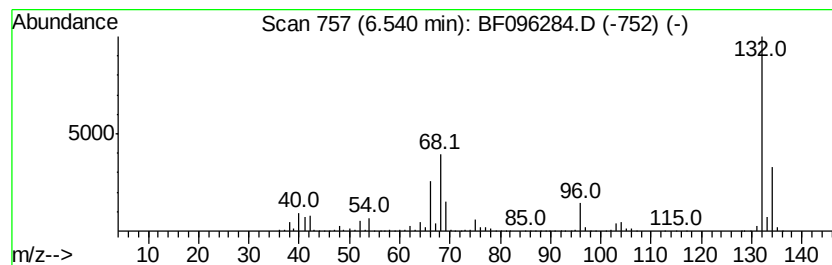
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Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	66.79 ng	3363150	1,4-Dichlorobenzene-d4	6.77

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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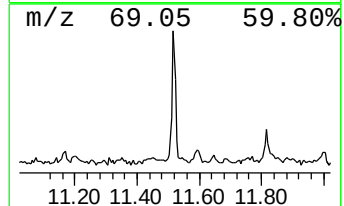
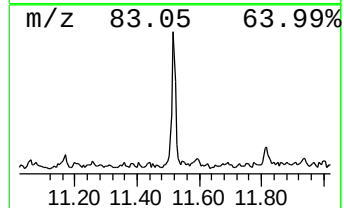
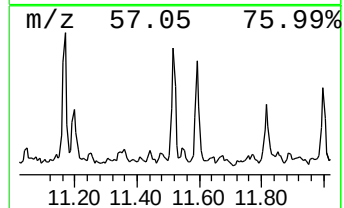
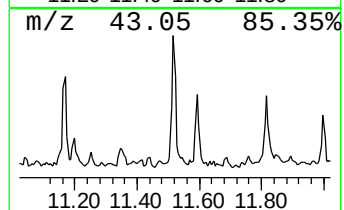
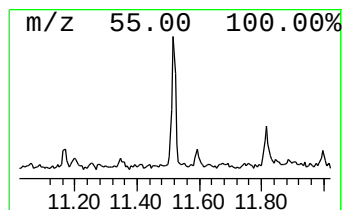
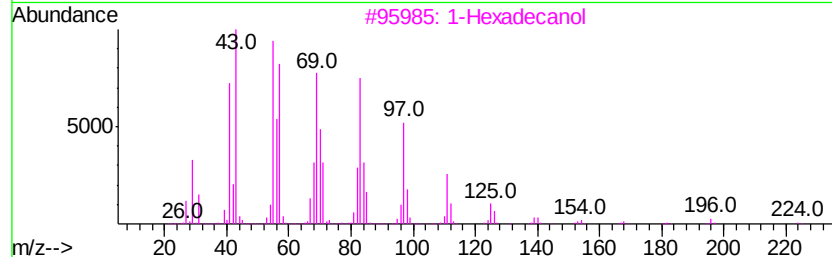
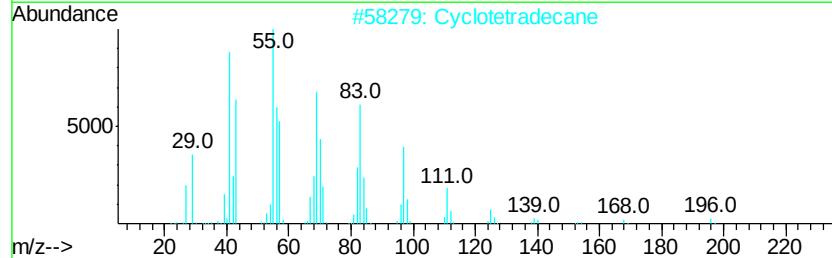
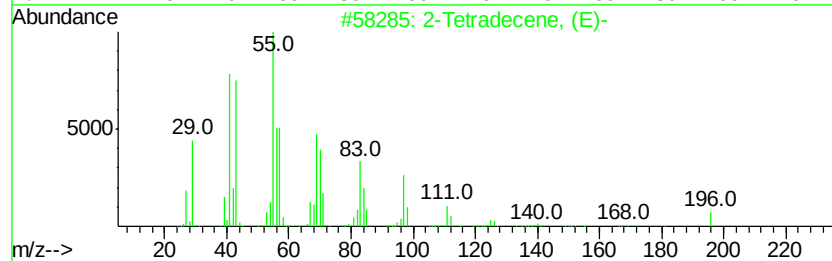
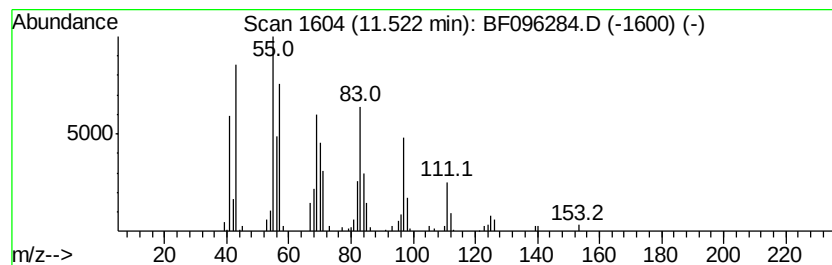
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Tetradecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.52	2.98 ng	176881	Phenanthrene-d10	11.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Tetradecene, (E)-	196	C14H28	035953-54-9	94
2	Cyclotetradecane	196	C14H28	000295-17-0	92
3	1-Hexadecanol	242	C16H34O	036653-82-4	91
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91



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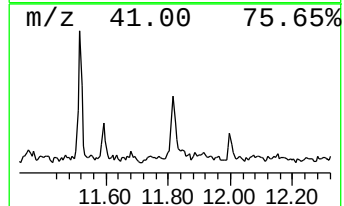
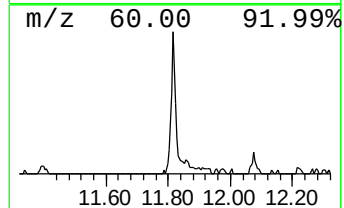
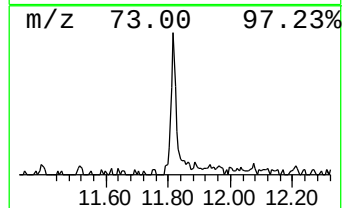
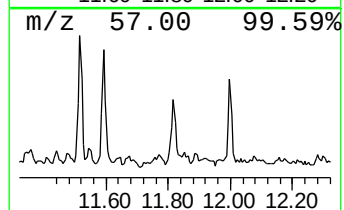
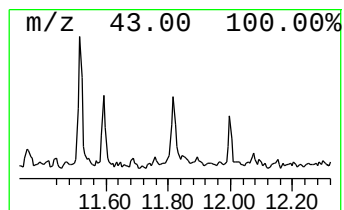
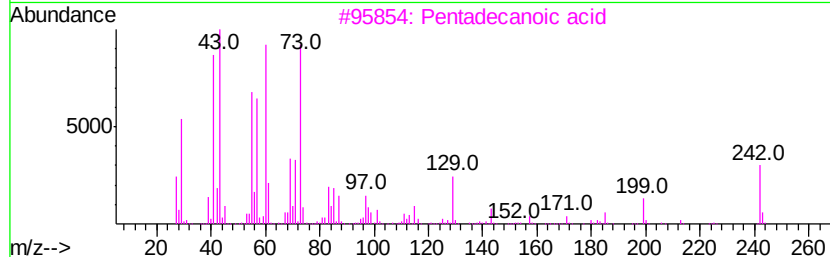
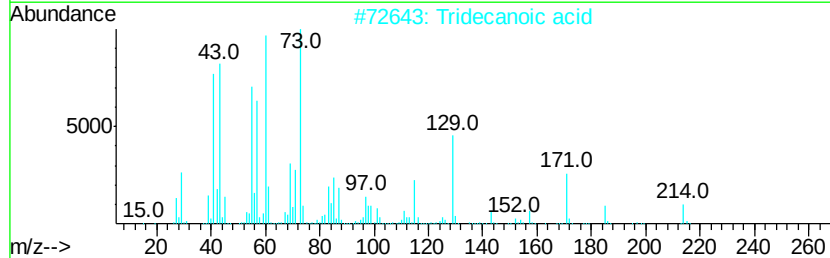
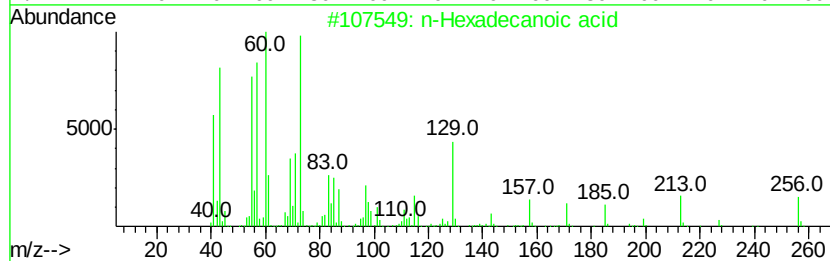
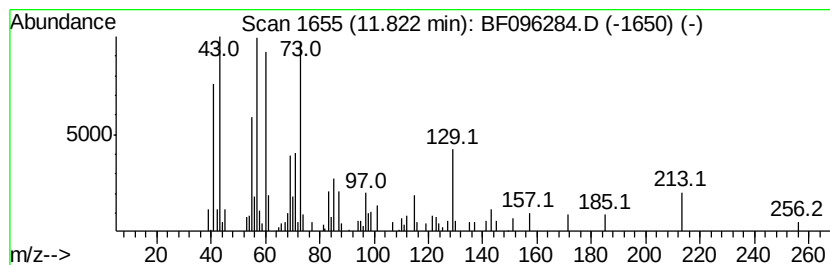
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.16 ng	128485	Phenanthrene-d10	11.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5		n-Decanoic acid	172	C10H20O2	000334-48-5	49



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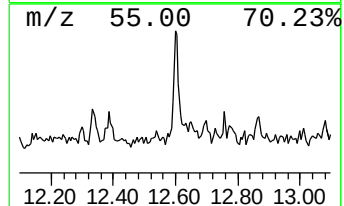
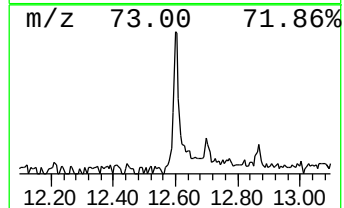
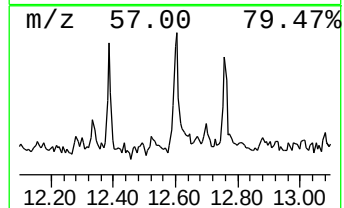
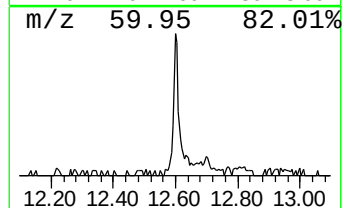
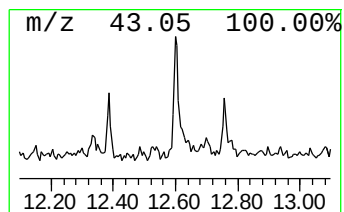
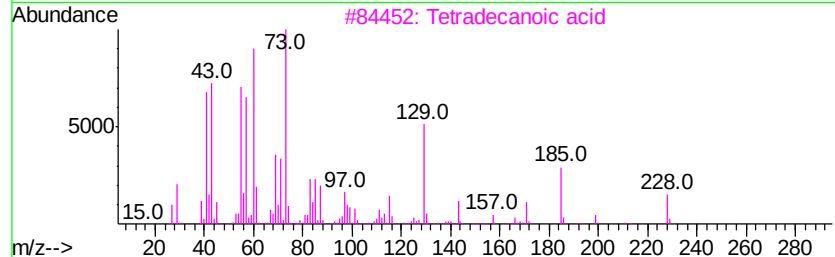
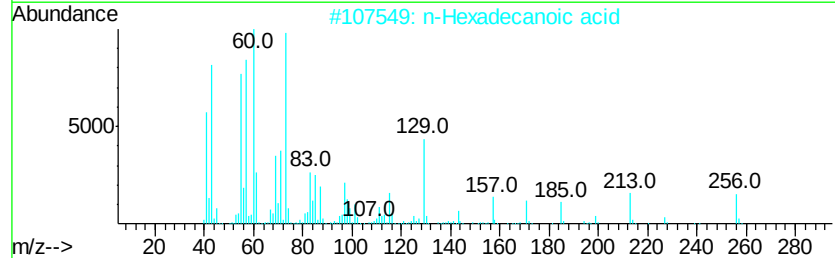
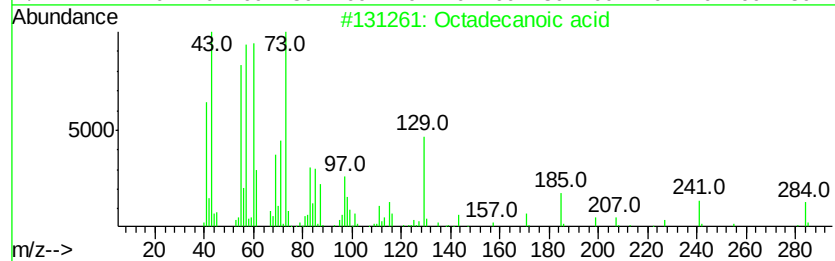
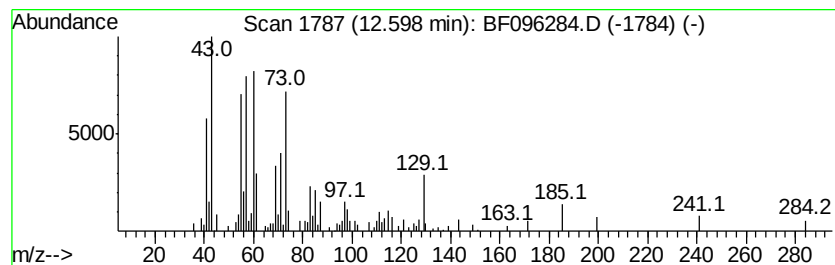
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	3.19 ng	141229	Chrysene-d12	13.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	87
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58



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ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

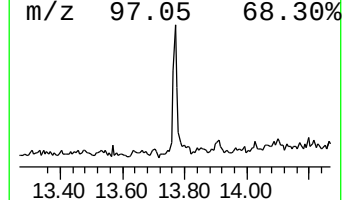
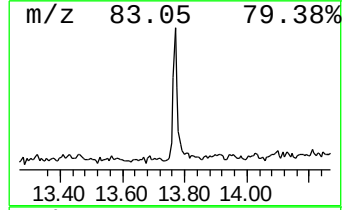
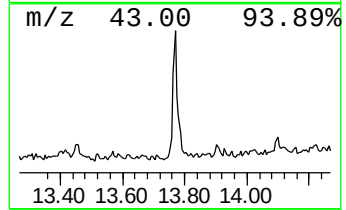
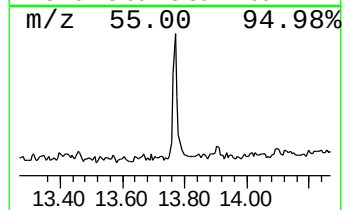
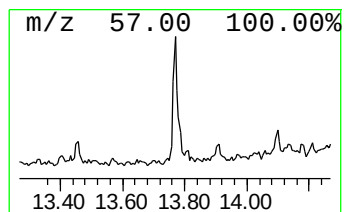
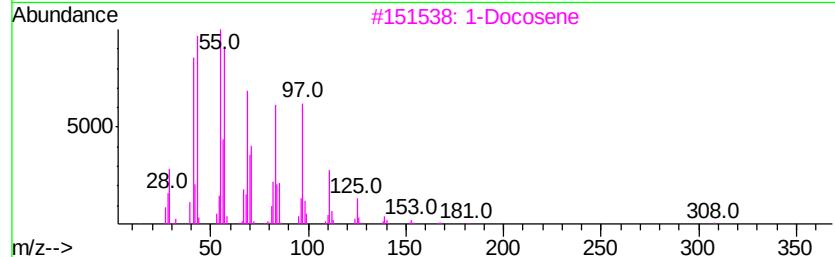
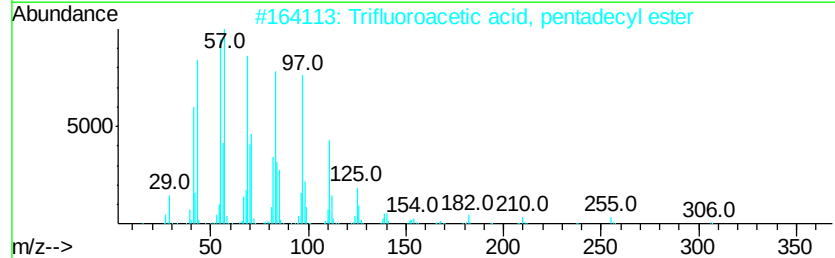
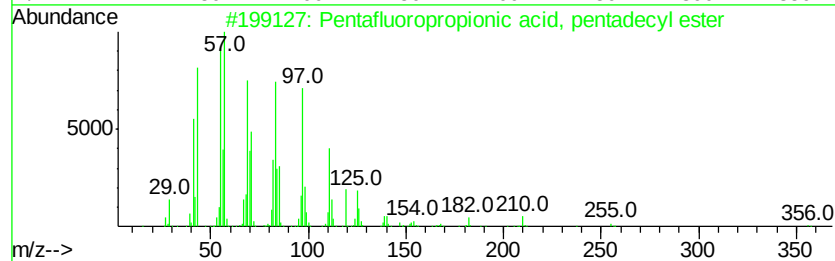
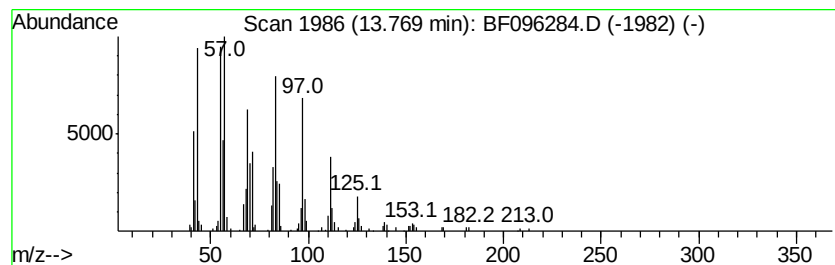
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	4.74 ng	209641	Chrysene-d12	13.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
3			1-Docosene	308	C22H44	001599-67-3	91
4			1-Heneicosanol	312	C21H44O	015594-90-8	91
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062917\
Data File : BF096284.D
Acq On : 29 Jun 2017 11:46
Operator : SJ/MA
Sample : I3899-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11940

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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
unknown4.97	4.97	14.9	ng	752056	1	6.77	1007090	20.0
unknown6.54	6.54	66.8	ng	3363150	1	6.77	1007090	20.0
2-Tetradecene, (E)-	11.52	3.0	ng	176881	4	11.28	1189040	20.0
n-Hexadecanoic acid	11.82	2.2	ng	128485	4	11.28	1189040	20.0
Octadecanoic acid	12.60	3.2	ng	141229	5	13.91	884942	20.0
Pentafluoropropio...	13.77	4.7	ng	209641	5	13.91	884942	20.0