

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
 Data File : BF099057.D
 Acq On : 4 Oct 2017 3:43
 Operator : SJ/JU
 Sample : I5588-02
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-ENV-114-4(0-5)

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	2.157	8	12	28	rVB	157688	293163	12.11%	1.313%
2	5.092	508	511	523	rVB	416748	528384	21.83%	2.367%
3	5.492	574	579	582	rBV	2465167	2322539	95.97%	10.402%
4	6.498	745	750	758	rVB	2138654	2354470	97.29%	10.545%
5	6.645	770	775	778	rBV	2462725	2419994	100.00%	10.839%
6	6.875	810	814	817	rVB	875562	718511	29.69%	3.218%
7	7.028	836	840	844	rBV	1984727	1873471	77.42%	8.391%
8	7.433	904	909	912	rBV	1489574	1466165	60.59%	6.567%
9	8.157	1027	1032	1035	rBV	984575	876460	36.22%	3.926%
10	9.227	1208	1214	1217	rBV	2676984	2280446	94.23%	10.214%
11	9.616	1277	1280	1284	rBV	337345	291105	12.03%	1.304%
12	9.910	1326	1330	1334	rVB	904169	754241	31.17%	3.378%
13	10.333	1399	1402	1405	rVB	36701	30393	1.26%	0.136%
14	10.698	1460	1464	1467	rBV	1018482	909309	37.57%	4.073%
15	10.804	1479	1482	1486	rBV	45958	42669	1.76%	0.191%
16	11.398	1579	1583	1585	rBV	683171	623376	25.76%	2.792%
17	11.416	1585	1586	1589	rVB	52446	35855	1.48%	0.161%
18	12.604	1785	1788	1792	rBV	109208	94241	3.89%	0.422%
19	12.792	1817	1820	1822	rBV	74998	59205	2.45%	0.265%
20	12.839	1822	1828	1831	rBV	102829	112339	4.64%	0.503%
21	12.980	1847	1852	1855	rBV	1766683	1675624	69.24%	7.505%
22	13.498	1936	1940	1942	rVB	56941	49332	2.04%	0.221%
23	13.862	1999	2002	2009	rVB2	110571	128289	5.30%	0.575%
24	14.033	2027	2031	2034	rBV	859351	806847	33.34%	3.614%
25	14.057	2034	2035	2040	rVB	80282	55947	2.31%	0.251%
26	14.186	2054	2057	2061	rBV	28930	33024	1.36%	0.148%
27	14.486	2105	2108	2111	rBV2	33742	39106	1.62%	0.175%
28	14.798	2158	2161	2166	rVB	28022	28684	1.19%	0.128%
29	15.074	2204	2208	2211	rBV	70445	97934	4.05%	0.439%
30	15.133	2215	2218	2224	rVB3	34341	42846	1.77%	0.192%
31	15.380	2257	2260	2265	rVB	42817	49971	2.06%	0.224%
32	15.445	2267	2271	2276	rVB	53320	73605	3.04%	0.330%
33	15.509	2277	2282	2293	rVB	598362	795337	32.87%	3.562%
34	15.956	2353	2358	2362	rBV	40903	54032	2.23%	0.242%

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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-BF092317.M
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35	16.462	2439	2444	2455	rVB3	41183	91037	3.76%	0.408%
36	16.986	2528	2533	2538	rVV3	22695	40435	1.67%	0.181%
37	17.062	2541	2546	2556	rVB3	32023	67134	2.77%	0.301%
38	17.433	2605	2609	2616	rVB	16317	31040	1.28%	0.139%
39	17.762	2661	2665	2674	rVB4	21936	52143	2.15%	0.234%
40	18.603	2804	2808	2815	rVB8	12756	28319	1.17%	0.127%

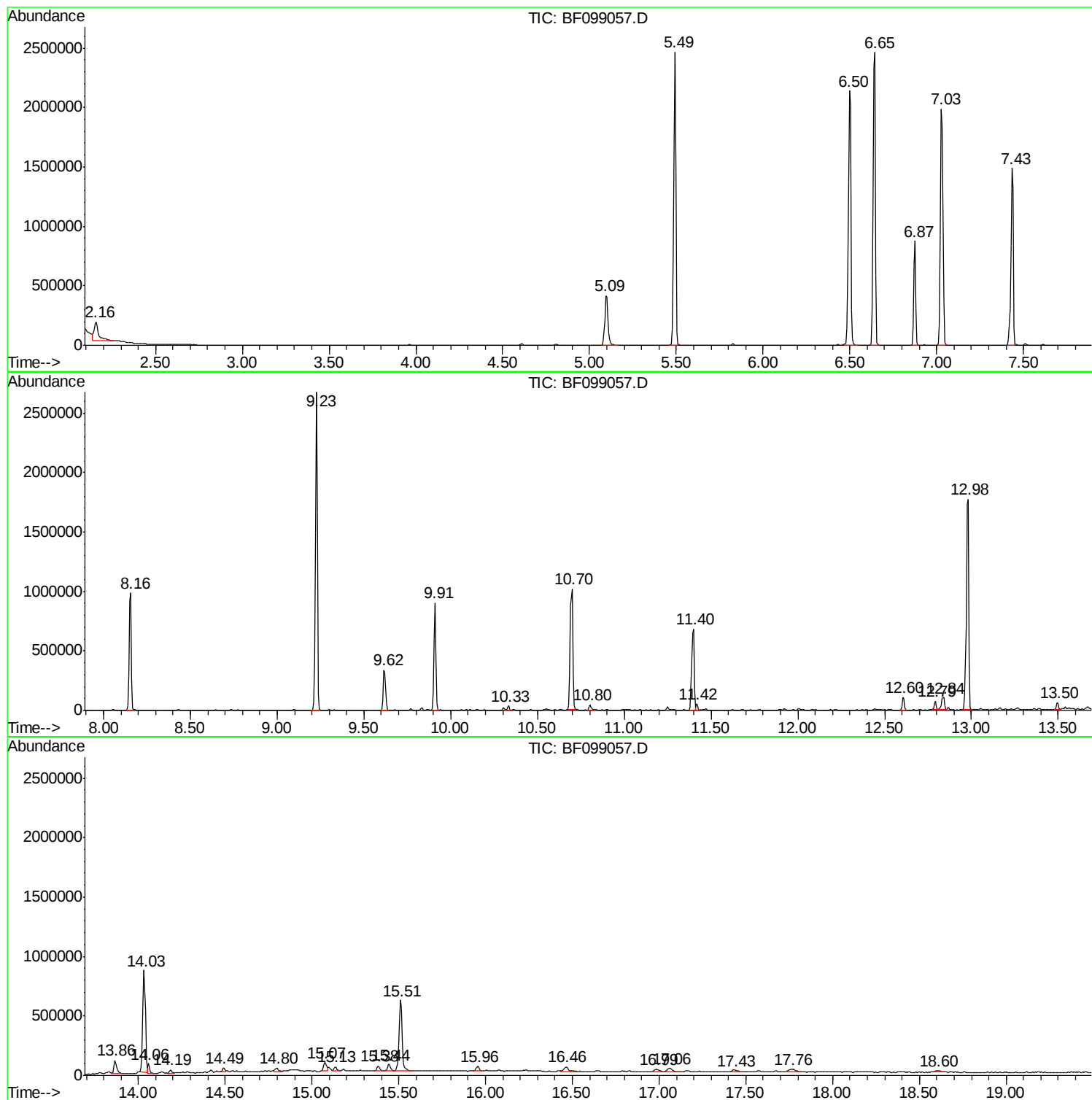
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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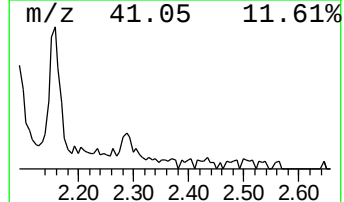
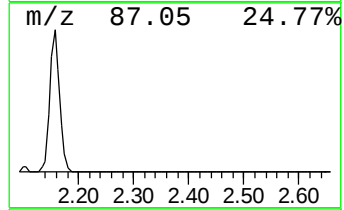
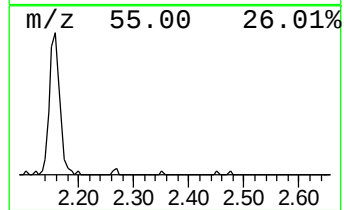
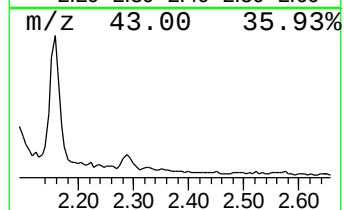
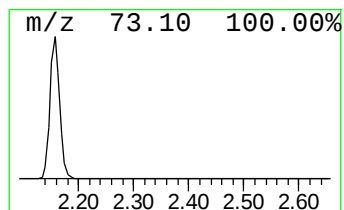
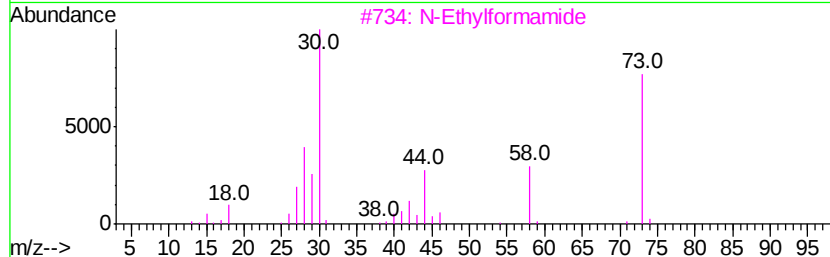
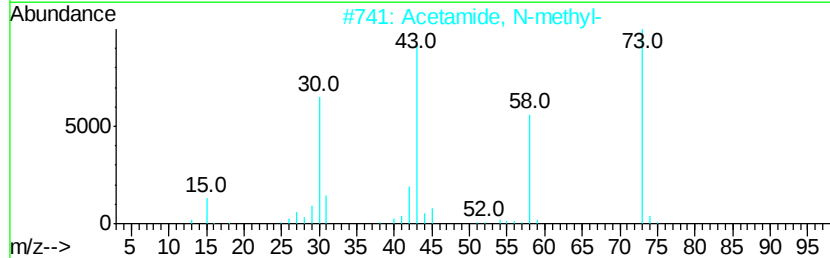
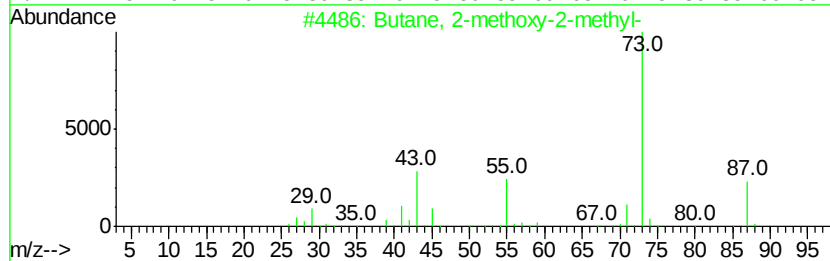
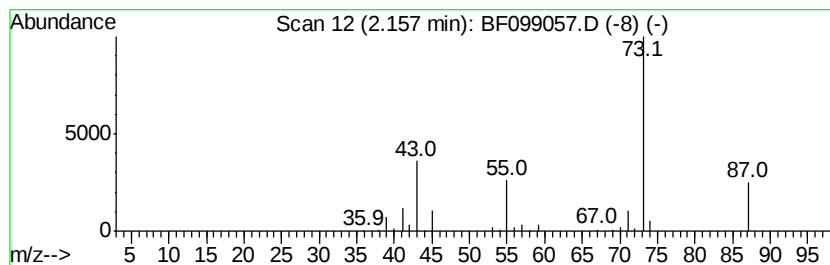
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	8.16 ng	293163	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	9



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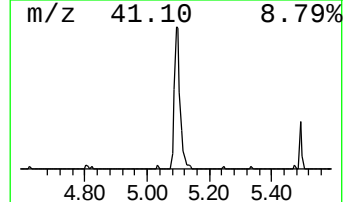
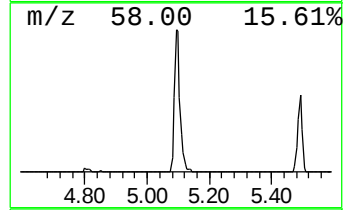
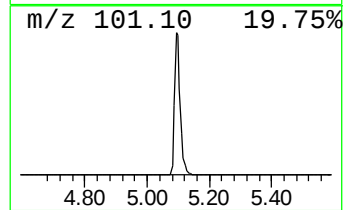
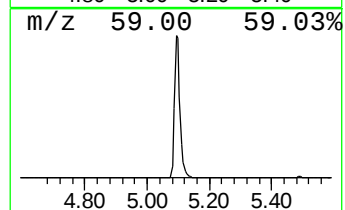
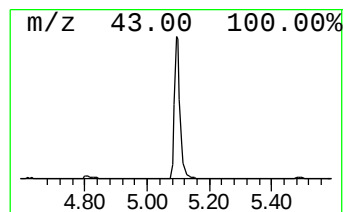
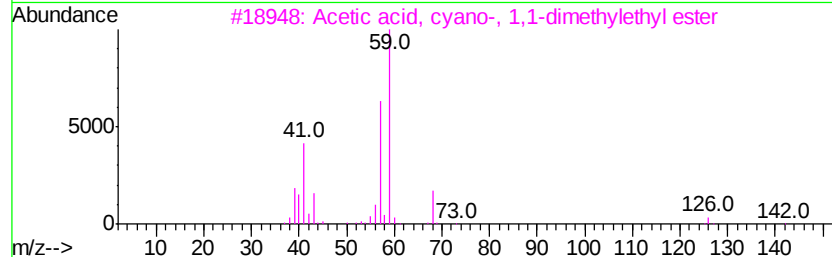
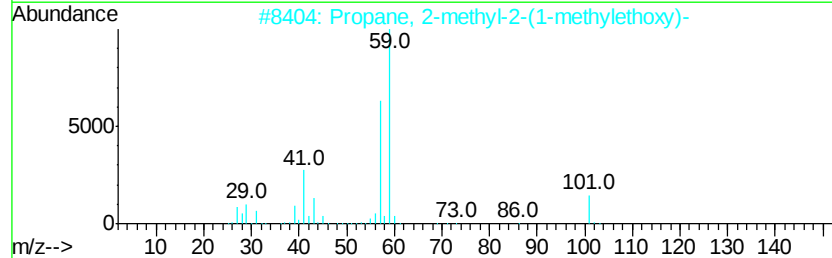
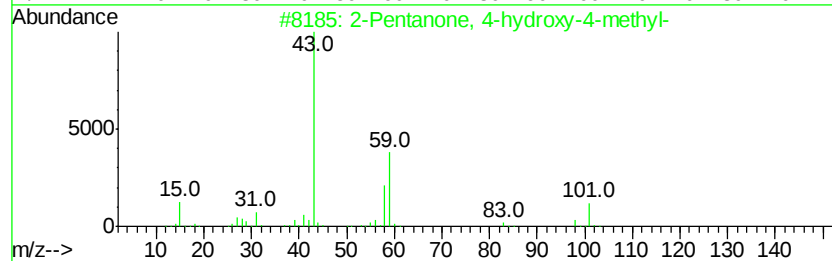
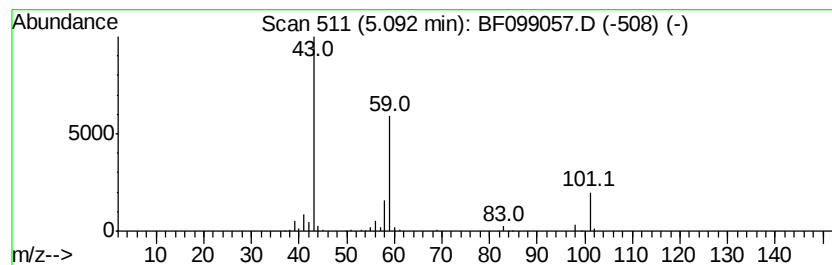
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	14.71 ng	528384	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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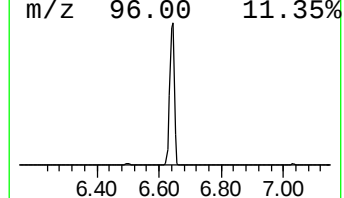
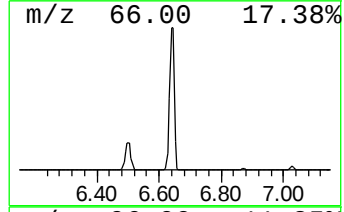
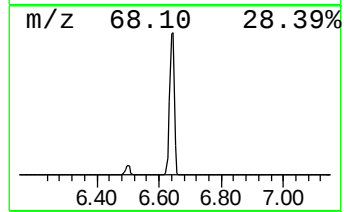
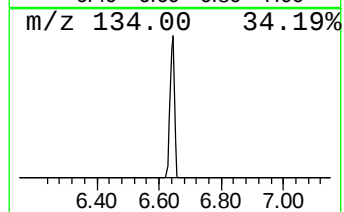
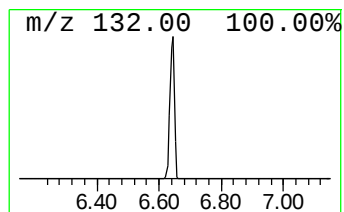
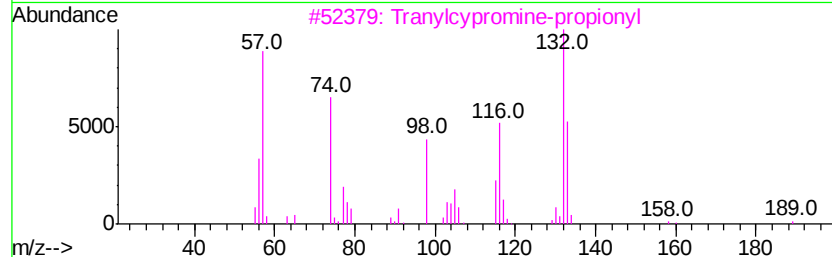
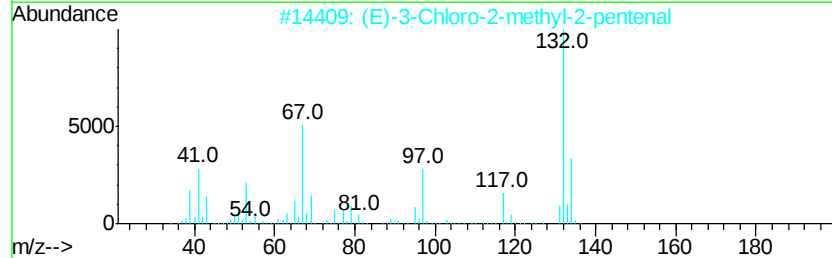
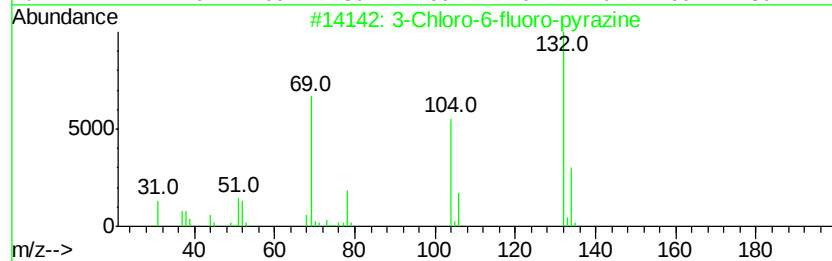
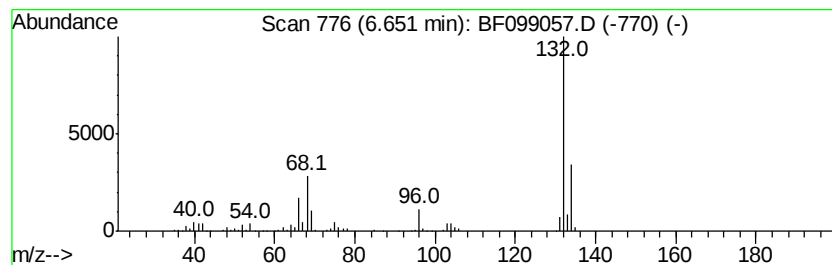
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	67.36 ng	2419990	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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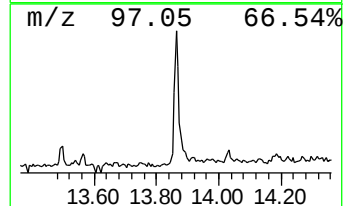
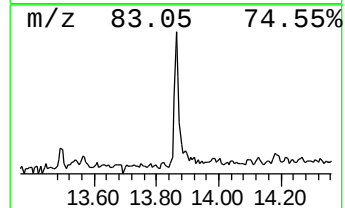
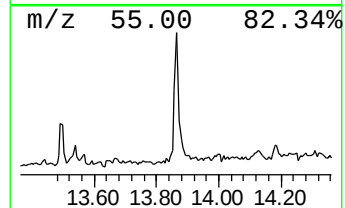
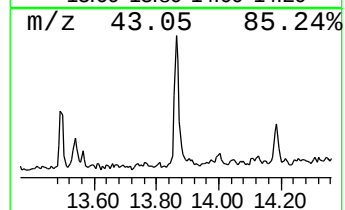
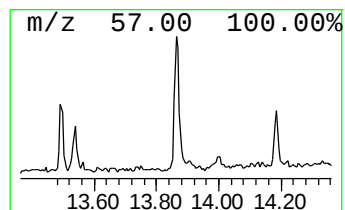
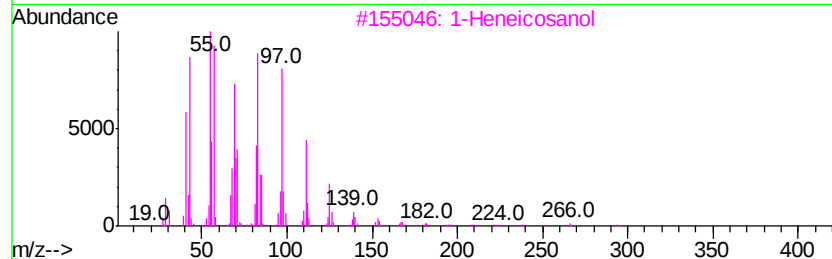
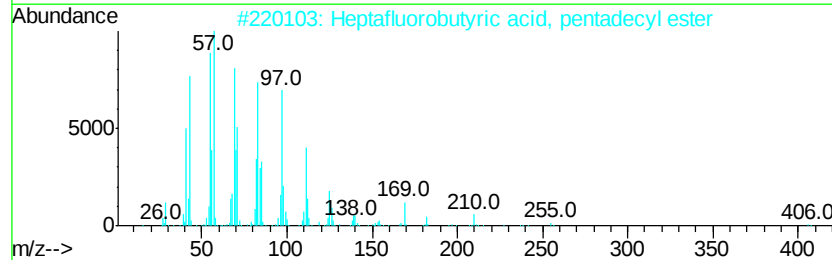
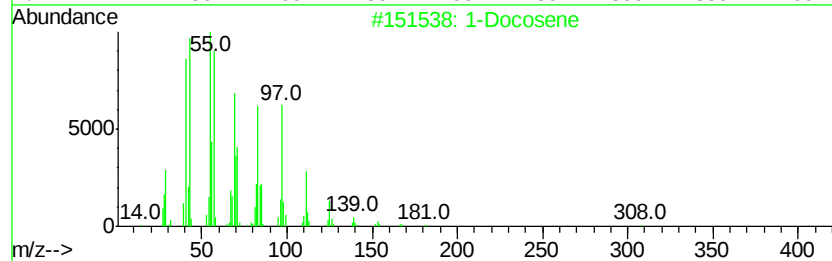
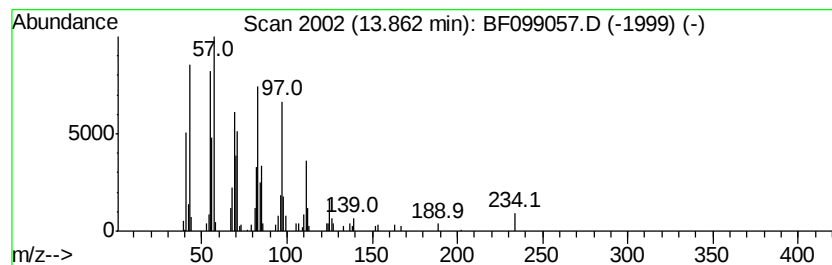
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TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.18 ng	128289	Chrysene-d12	14.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene		308 C22H44	001599-67-3 94
2	Heptafluorobutyric acid, pentade...		424 C19H31F7O2	959261-23-5 93
3	1-Heneicosanol		312 C21H44O	015594-90-8 93
4	Trifluoroacetoxy hexadecane		338 C18H33F3O2	006222-03-3 91
5	2- Bromopropionic acid, pentadec...		362 C18H35BrO2	1000292-44-2 91



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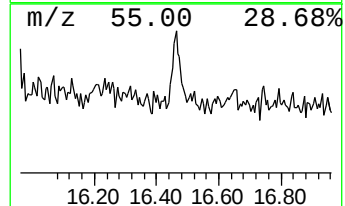
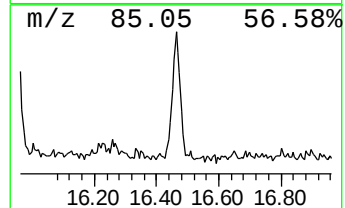
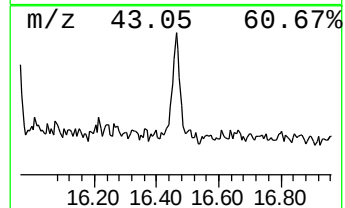
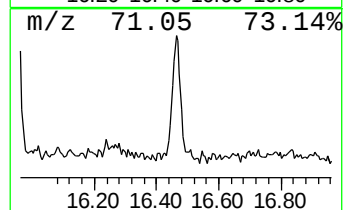
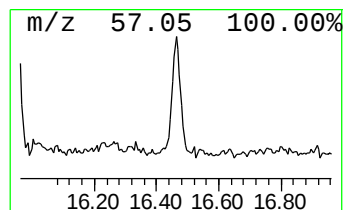
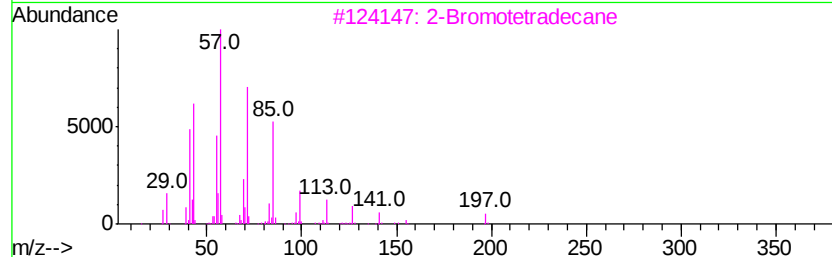
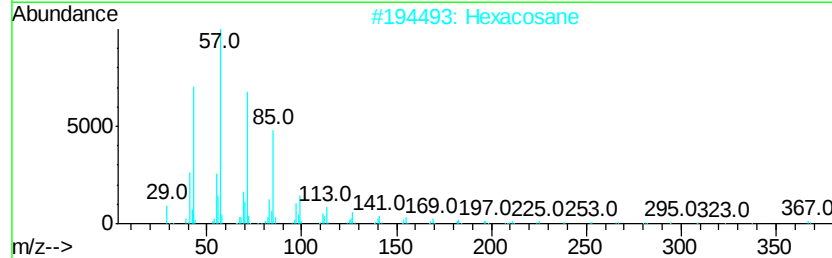
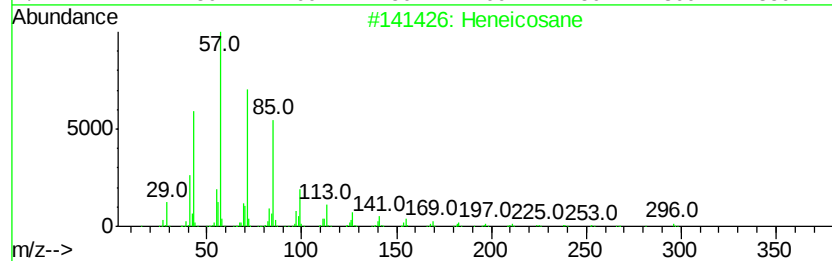
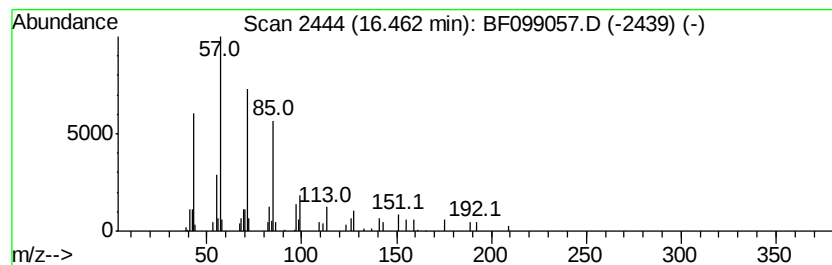
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	2.29 ng	91037	Perylene-d12	15.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	87
2	Hexacosane		366	C26H54	000630-01-3	86
3	2-Bromotetradecane		276	C14H29Br	074036-95-6	86
4	Heptadecane		240	C17H36	000629-78-7	86
5	Hentriacontane		437	C31H64	000630-04-6	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099057.D
Acq On : 4 Oct 2017 3:43
Operator : SJ/JU
Sample : I5588-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-114-4(0-5)

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...	2.16	8.2	ng	293163	1	6.87	718511	20.0
2-Pentanone, 4-hy...	5.09	14.7	ng	528384	1	6.87	718511	20.0
unknown6.65	6.65	67.4	ng	2419990	1	6.87	718511	20.0
1-Docosene	13.86	3.2	ng	128289	5	14.03	806847	20.0
Heneicosane	16.46	2.3	ng	91037	6	15.51	795337	20.0