

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
 Data File : BF098564.D
 Acq On : 15 Sep 2017 12:47
 Operator : SJ/JU
 Sample : I5188-11
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RL-2-17.25-34.5

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-BF091117.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	3.534	240	246	254	rBV	60127	104245	2.98%	0.353%
2	4.822	461	465	479	rBV	205222	302280	8.63%	1.023%
3	5.257	534	539	556	rBV	2797821	3126664	89.28%	10.580%
4	6.298	712	716	732	rBV	2808835	3280199	93.66%	11.100%
5	6.416	732	736	740	rBV	3368662	3203912	91.49%	10.842%
6	6.640	771	774	783	rBV	847002	810425	23.14%	2.742%
7	6.798	797	801	808	rBV	2797640	2428175	69.33%	8.217%
8	7.216	867	872	875	rBV	1976436	1980741	56.56%	6.703%
9	7.245	875	877	883	rVB2	47822	50481	1.44%	0.171%
10	7.928	988	993	996	rBV	1261893	1108278	31.65%	3.750%
11	8.639	1112	1114	1118	rVB	41217	36534	1.04%	0.124%
12	9.004	1171	1176	1179	rBV	3777312	3502092	100.00%	11.851%
13	9.086	1185	1190	1196	rVB2	39838	44131	1.26%	0.149%
14	9.404	1240	1244	1247	rBV	435204	357592	10.21%	1.210%
15	9.616	1277	1280	1283	rVB	61232	49475	1.41%	0.167%
16	9.680	1283	1291	1295	rBV	1250592	1141498	32.59%	3.863%
17	10.116	1361	1365	1367	rVB	71235	59859	1.71%	0.203%
18	10.333	1396	1402	1405	rBV	27604	37889	1.08%	0.128%
19	10.469	1421	1425	1429	rBV	1665420	1487126	42.46%	5.032%
20	10.586	1442	1445	1453	rVB	113946	119027	3.40%	0.403%
21	11.033	1518	1521	1524	rBV	59972	49754	1.42%	0.168%
22	11.163	1539	1543	1545	rBV	1187838	1030854	29.44%	3.488%
23	11.186	1545	1547	1550	rVB	103321	86079	2.46%	0.291%
24	12.210	1719	1721	1724	rBV2	31762	36883	1.05%	0.125%
25	12.374	1745	1749	1752	rBV	118334	114801	3.28%	0.388%
26	12.598	1784	1787	1790	rVV	92986	70545	2.01%	0.239%
27	12.633	1790	1793	1803	rVB2	89299	133003	3.80%	0.450%
28	12.745	1808	1812	1816	rBV	2609949	2594011	74.07%	8.778%
29	13.645	1962	1965	1970	rBV2	224795	231144	6.60%	0.782%
30	13.798	1987	1991	1994	rBV	841202	804513	22.97%	2.722%
31	14.274	2069	2072	2075	rBV2	55125	70545	2.01%	0.239%
32	14.698	2142	2144	2148	rVB3	57519	46168	1.32%	0.156%
33	14.874	2171	2174	2176	rBV	51886	51540	1.47%	0.174%
34	15.198	2225	2229	2238	rVB	640998	819695	23.41%	2.774%

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Smoothing : ON Filtering: 5
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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	15.398	2260	2263	2272	rVB4	72955	118118	3.37%	0.400%
36	15.604	2296	2298	2302	rVB	52672	63137	1.80%	0.214%

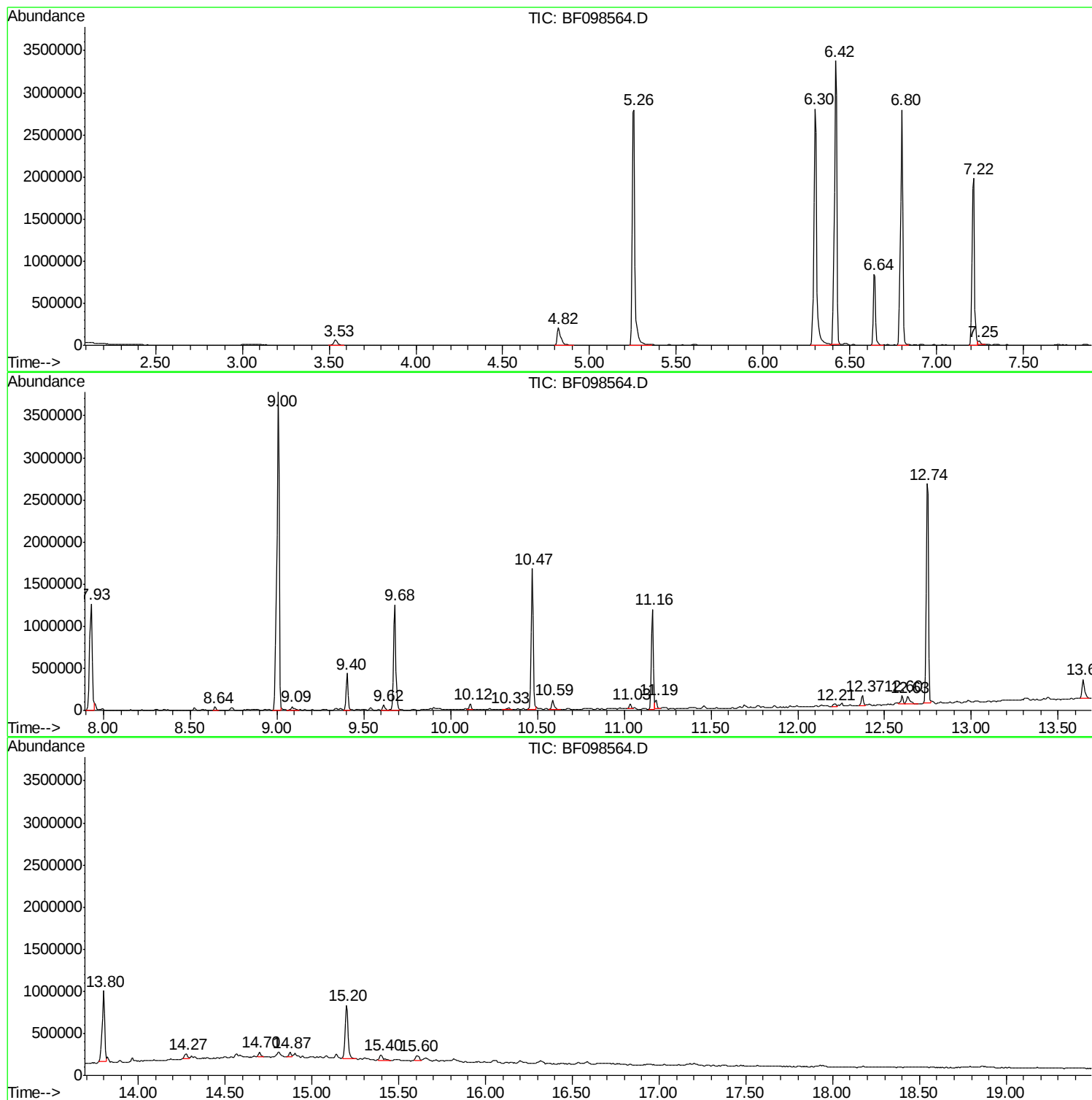
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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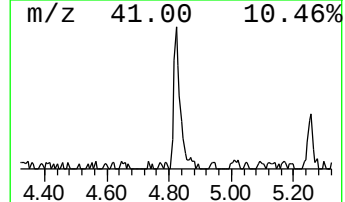
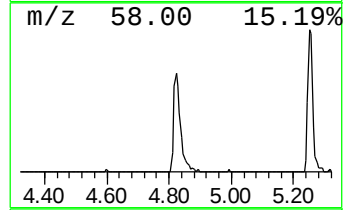
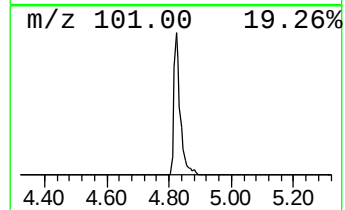
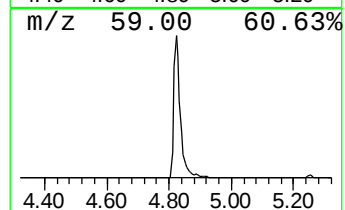
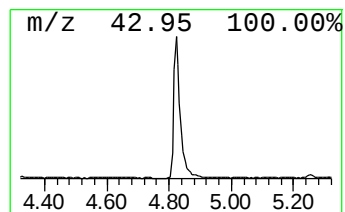
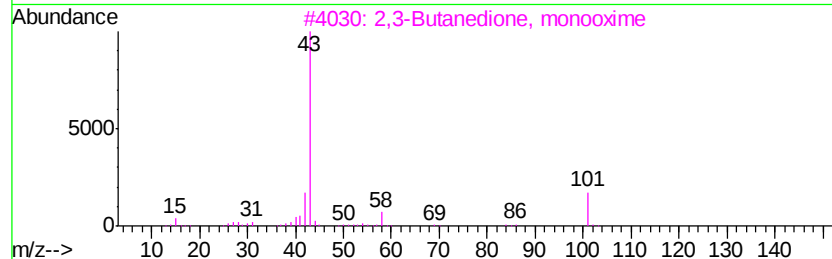
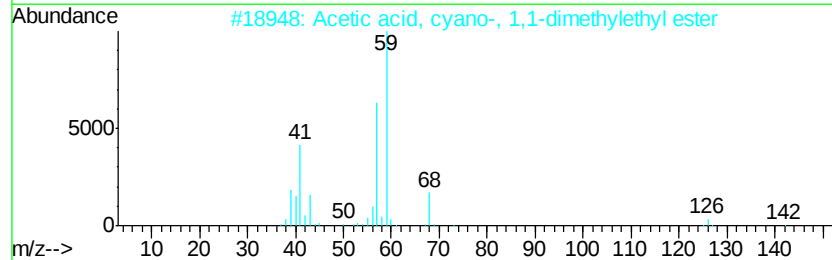
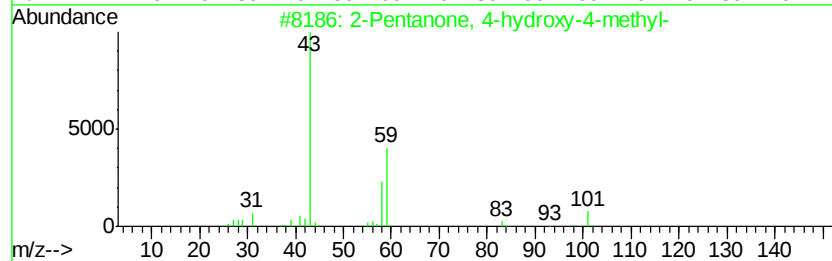
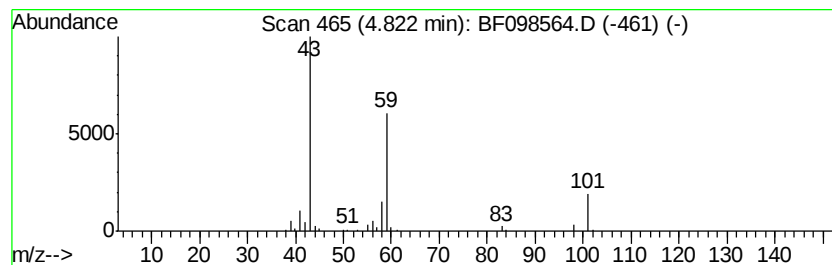
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	7.46 ng	302280	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		3-Hexanol	102	C6H14O	000623-37-0	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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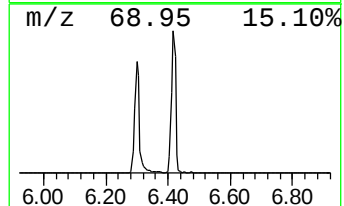
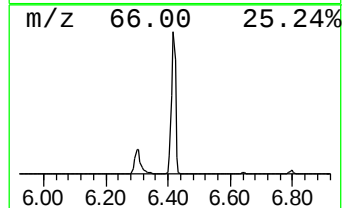
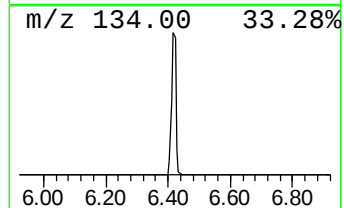
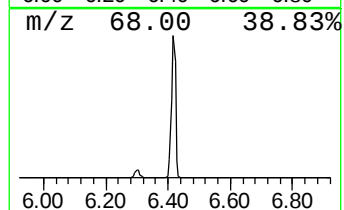
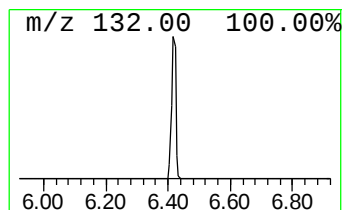
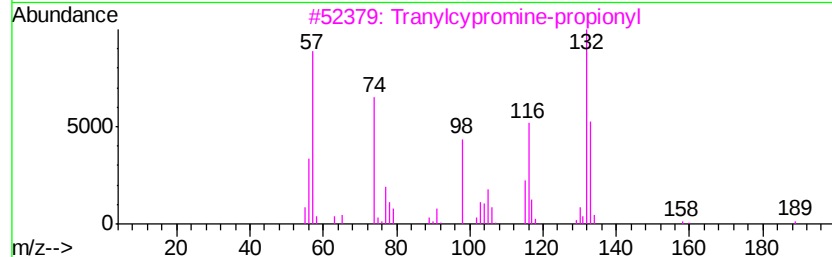
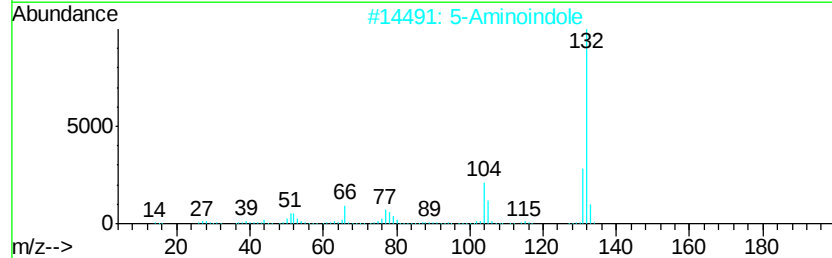
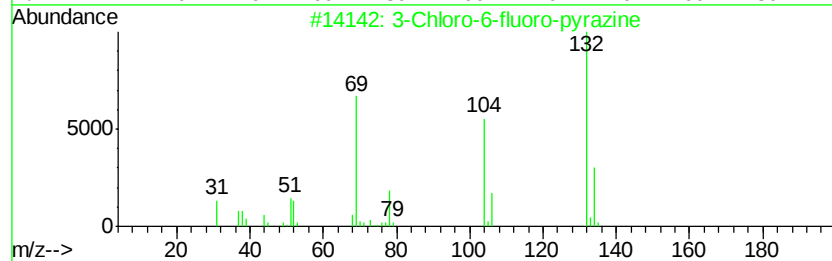
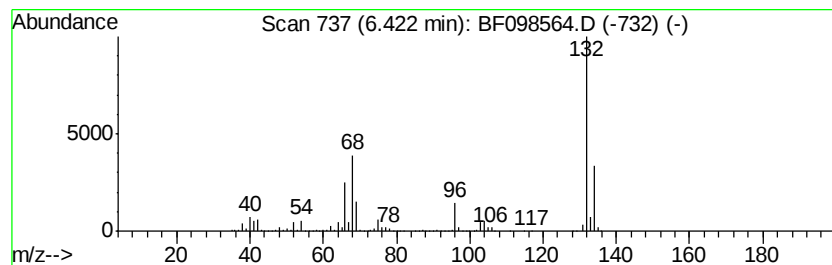
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	79.07 ng	3203910	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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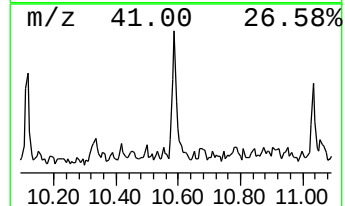
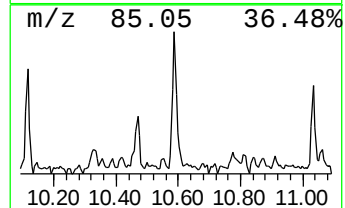
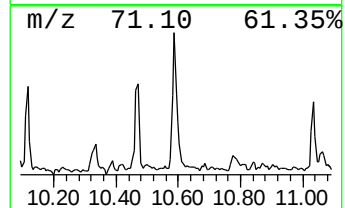
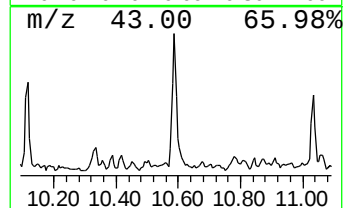
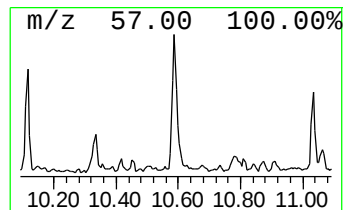
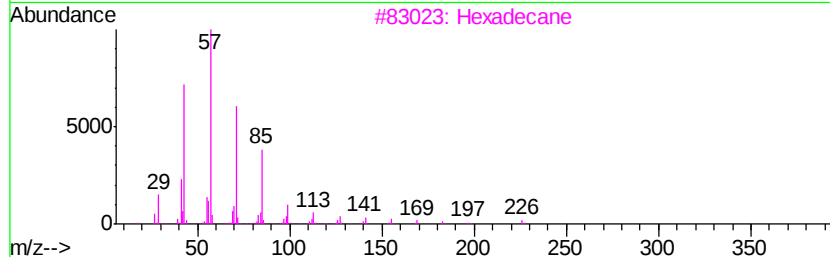
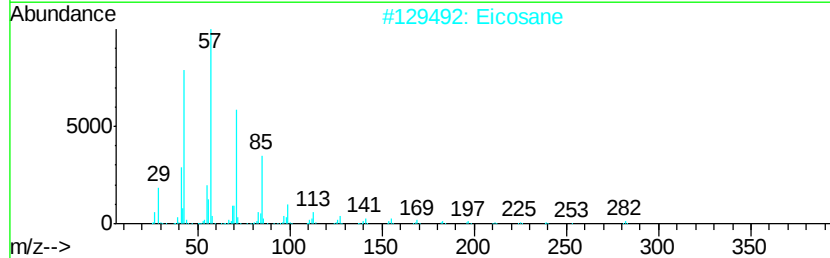
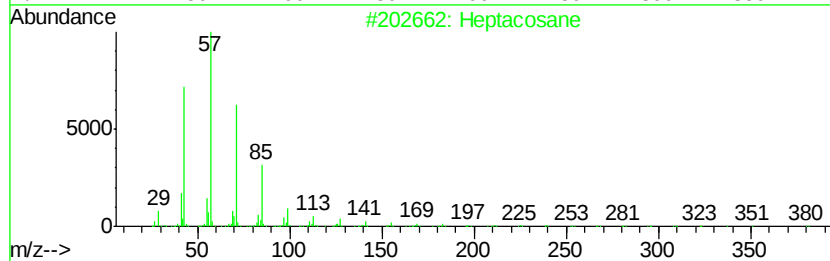
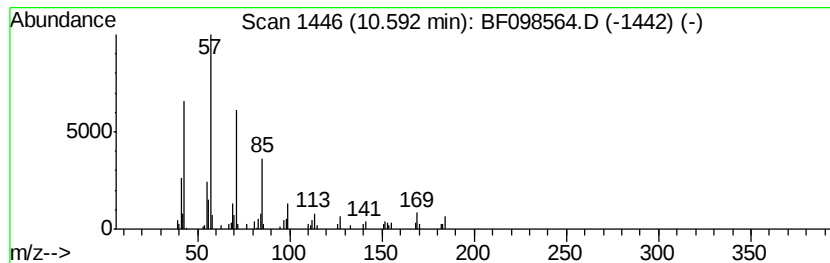
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	2.31 ng	119027	Phenanthrene-d10	11.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Eicosane		282	C20H42	000112-95-8	91
3	Hexadecane		226	C16H34	000544-76-3	90
4	Pentadecane		212	C15H32	000629-62-9	90
5	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	87



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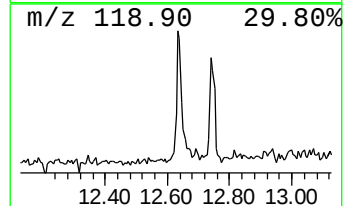
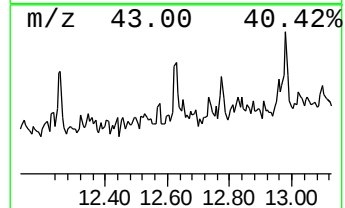
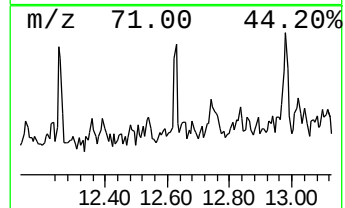
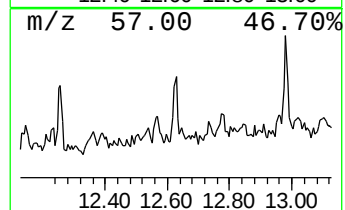
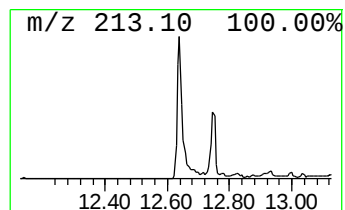
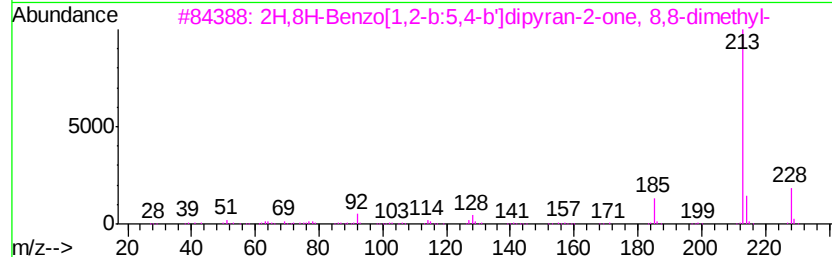
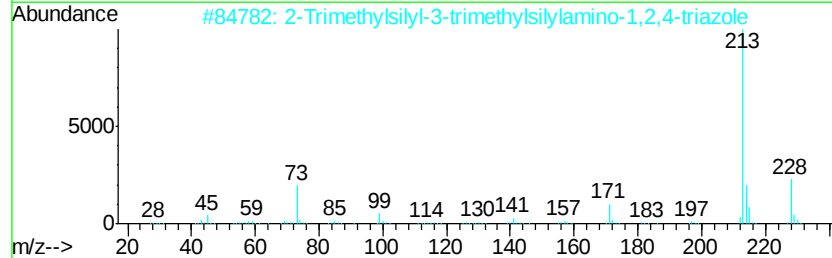
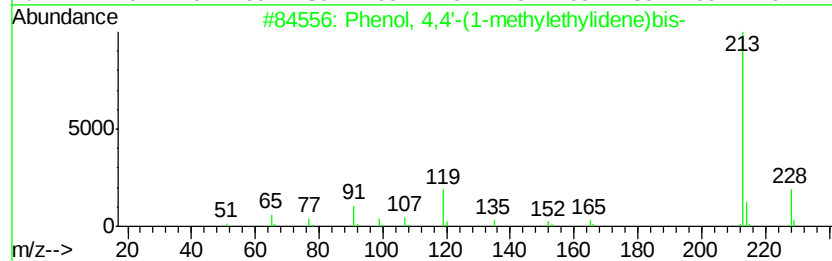
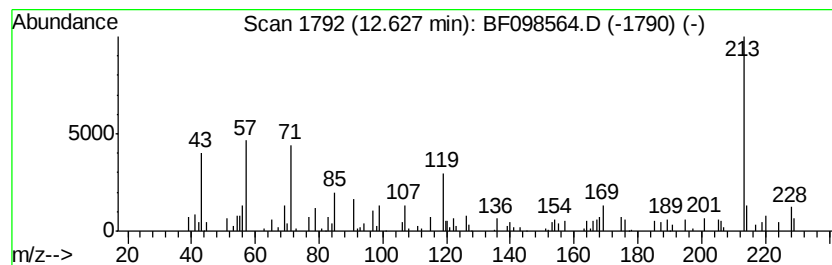
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	3.31 ng	133003	Chrysene-d12	13.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	93
2		2-Trimethylsilyl-3-trimethylsilyl...	228	C8H20N4Si2	1000373-05-5	64
3		2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	58
4		2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	53
5		Indole,6-methyl-2-(2-thienyl)-	213	C13H11NS	296245-70-0	50



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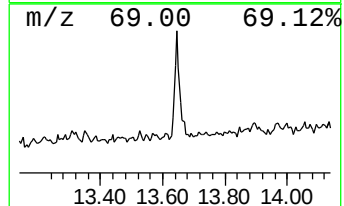
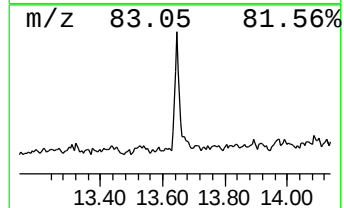
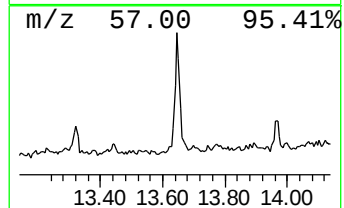
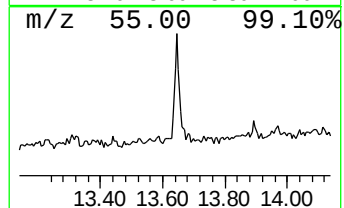
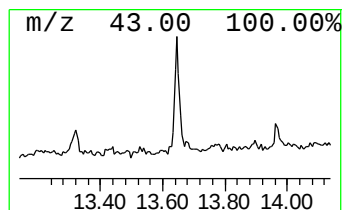
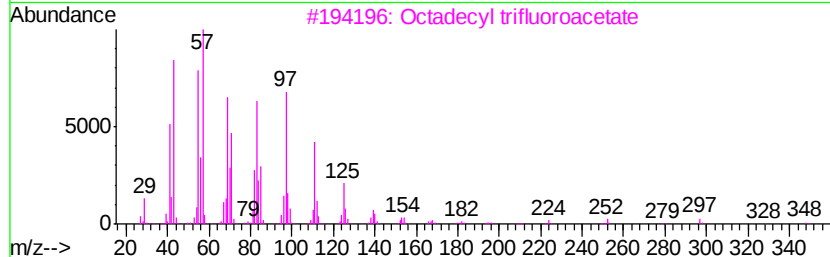
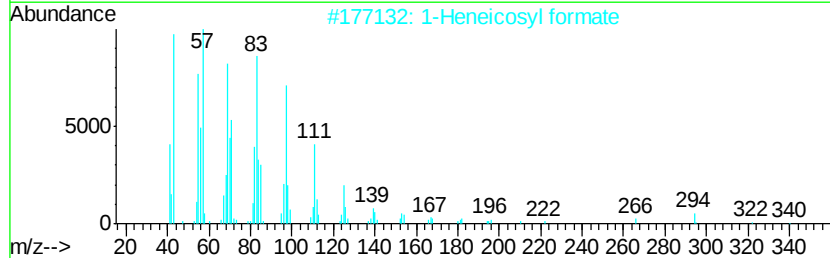
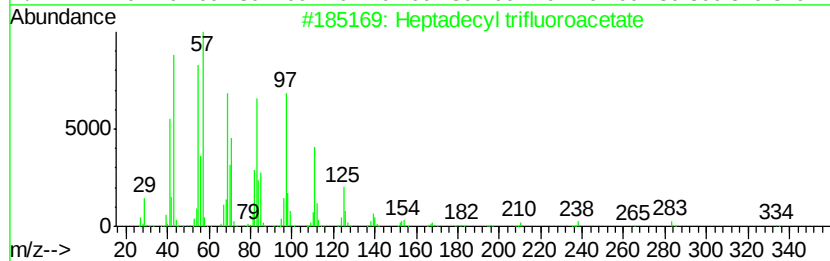
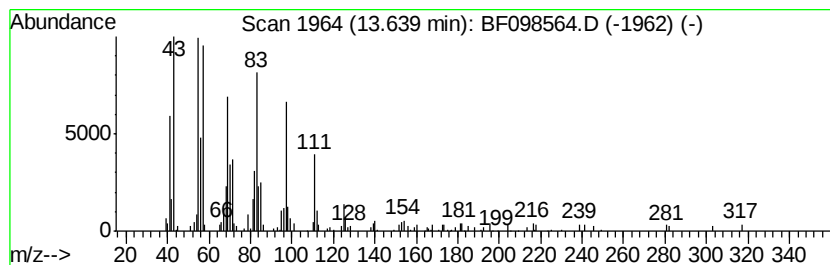
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Peak Number 7 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	5.75 ng	231144	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098564.D
Acq On : 15 Sep 2017 12:47
Operator : SJ/JU
Sample : I5188-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RL-2-17.25-34.5

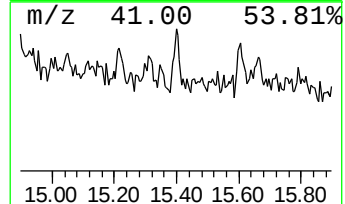
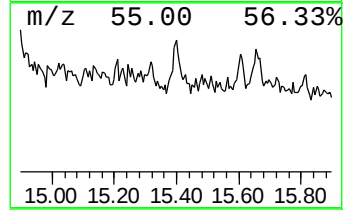
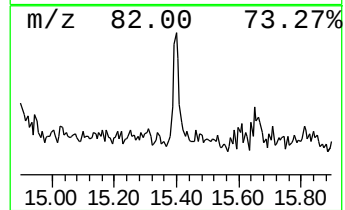
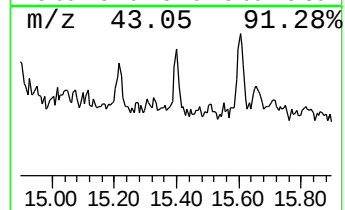
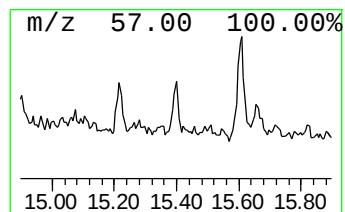
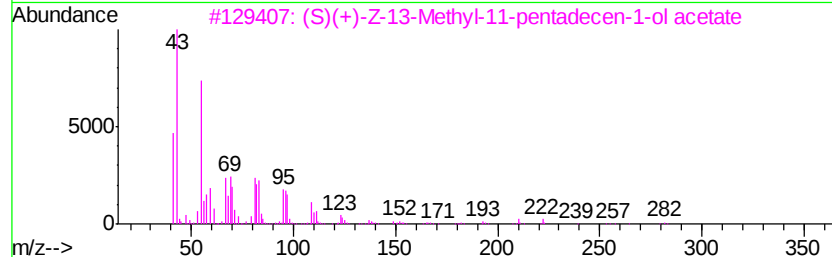
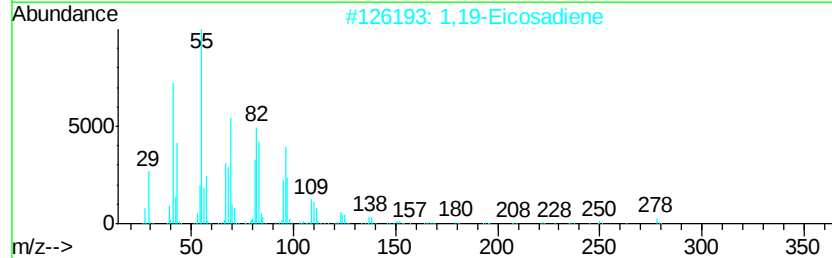
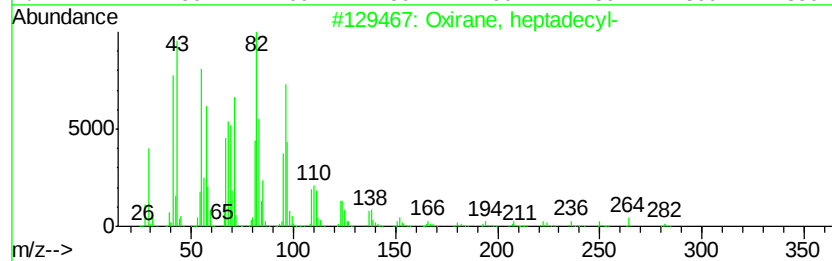
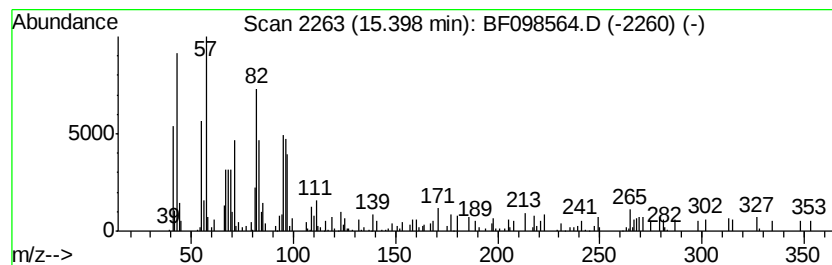
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, heptadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	2.88 ng	118118	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	89
2		1,19-Eicosadiene	278	C20H38	014811-95-1	52
3		(S)(+)-Z-13-Methyl-11-pentadecen...	282	C18H34O2	1000130-84-8	47
4		Oxirane, tetradecyl-	240	C16H32O	007320-37-8	46
5		9-Octadecen-1-ol, (E)-	268	C18H36O	000506-42-3	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098564.D
Acq On : 15 Sep 2017 12:47
Operator : SJ/JU
Sample : I5188-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RL-2-17.25-34.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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...	4.82	7.5	ng	302280	1	6.65	810425	20.0
unknown6.42	6.42	79.1	ng	3203910	1	6.65	810425	20.0
Heptacosane	10.59	2.3	ng	119027	4	11.16	1030850	20.0
Phenol, 4,4'-(1-m...	12.63	3.3	ng	133003	5	13.80	804513	20.0
Heptadecyl triflu...	13.64	5.8	ng	231144	5	13.80	804513	20.0
Oxirane, heptadecyl-	15.40	2.9	ng	118118	6	15.20	819695	20.0