

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
 Data File : BF097449.D
 Acq On : 8 Aug 2017 00:37
 Operator : SJ/JU
 Sample : I4582-02
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S2

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	4.522	462	465	477	rBV	139404	216091	17.68%	1.706%
2	5.004	544	547	570	rBV	831381	1154446	94.46%	9.115%
3	6.081	727	730	744	rBV	1025380	1222178	100.00%	9.650%
4	6.187	744	748	765	rVB	1166335	1209936	99.00%	9.553%
5	6.410	783	786	800	rVB	606945	552809	45.23%	4.365%
6	6.563	809	812	823	rBV	896580	880252	72.02%	6.950%
7	6.981	880	883	901	rBV	807312	792615	64.85%	6.258%
8	7.692	1001	1004	1024	rVB	851224	764110	62.52%	6.033%
9	8.769	1184	1187	1197	rBV	1236996	1090701	89.24%	8.612%
10	9.175	1252	1256	1264	rBV	205367	174069	14.24%	1.374%
11	9.433	1297	1300	1310	rVB	667918	649326	53.13%	5.127%
12	9.892	1375	1378	1381	rVB	19038	15181	1.24%	0.120%
13	10.222	1431	1434	1447	rBV	530887	513973	42.05%	4.058%
14	10.363	1455	1458	1464	rBV	30013	36000	2.95%	0.284%
15	10.804	1530	1533	1536	rBV	16532	14945	1.22%	0.118%
16	10.910	1547	1551	1554	rBV	595947	522546	42.76%	4.126%
17	10.933	1554	1555	1559	rVB	30769	20073	1.64%	0.158%
18	11.433	1638	1640	1644	rBV3	11988	14181	1.16%	0.112%
19	11.469	1644	1646	1653	rVB4	44639	46557	3.81%	0.368%
20	12.116	1753	1756	1760	rBV	78771	68114	5.57%	0.538%
21	12.339	1789	1794	1798	rBV	94092	90466	7.40%	0.714%
22	12.492	1816	1820	1823	rVB	858990	789978	64.64%	6.237%
23	12.739	1859	1862	1866	rBV3	11837	14353	1.17%	0.113%
24	13.427	1972	1979	1992	rBV5	44268	104764	8.57%	0.827%
25	13.533	1992	1997	2000	rVV	657865	646957	52.93%	5.108%
26	13.557	2000	2001	2005	rVB	48941	41818	3.42%	0.330%
27	13.639	2010	2015	2018	rBV4	13186	15095	1.24%	0.119%
28	13.927	2061	2064	2067	rBV3	15666	21467	1.76%	0.169%
29	14.063	2083	2087	2097	rVB7	33137	65203	5.33%	0.515%
30	14.251	2115	2119	2122	rBV4	14721	23871	1.95%	0.188%
31	14.321	2128	2131	2134	rBV3	12327	15743	1.29%	0.124%
32	14.445	2149	2152	2157	rBV3	45088	47561	3.89%	0.376%
33	14.527	2163	2166	2174	rBV	42382	72146	5.90%	0.570%
34	14.604	2176	2179	2183	rBV2	37378	46339	3.79%	0.366%

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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

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35	14.657	2184	2188	2194	rVB5	27100	52646	4.31%	0.416%
36	14.774	2205	2208	2213	rVB	24274	26031	2.13%	0.206%
37	14.827	2213	2217	2221	rBV	31409	37415	3.06%	0.295%
38	14.874	2221	2225	2229	rBV	344079	383687	31.39%	3.029%
39	15.068	2255	2258	2262	rVB4	25422	33437	2.74%	0.264%
40	15.115	2262	2266	2270	rBV7	13775	35793	2.93%	0.283%
41	15.251	2285	2289	2296	rVB2	48165	64763	5.30%	0.511%
42	15.574	2342	2344	2347	rBV3	12645	18131	1.48%	0.143%
43	15.651	2353	2357	2362	rVB4	17903	26541	2.17%	0.210%
44	16.080	2425	2430	2431	rBV2	20216	33027	2.70%	0.261%

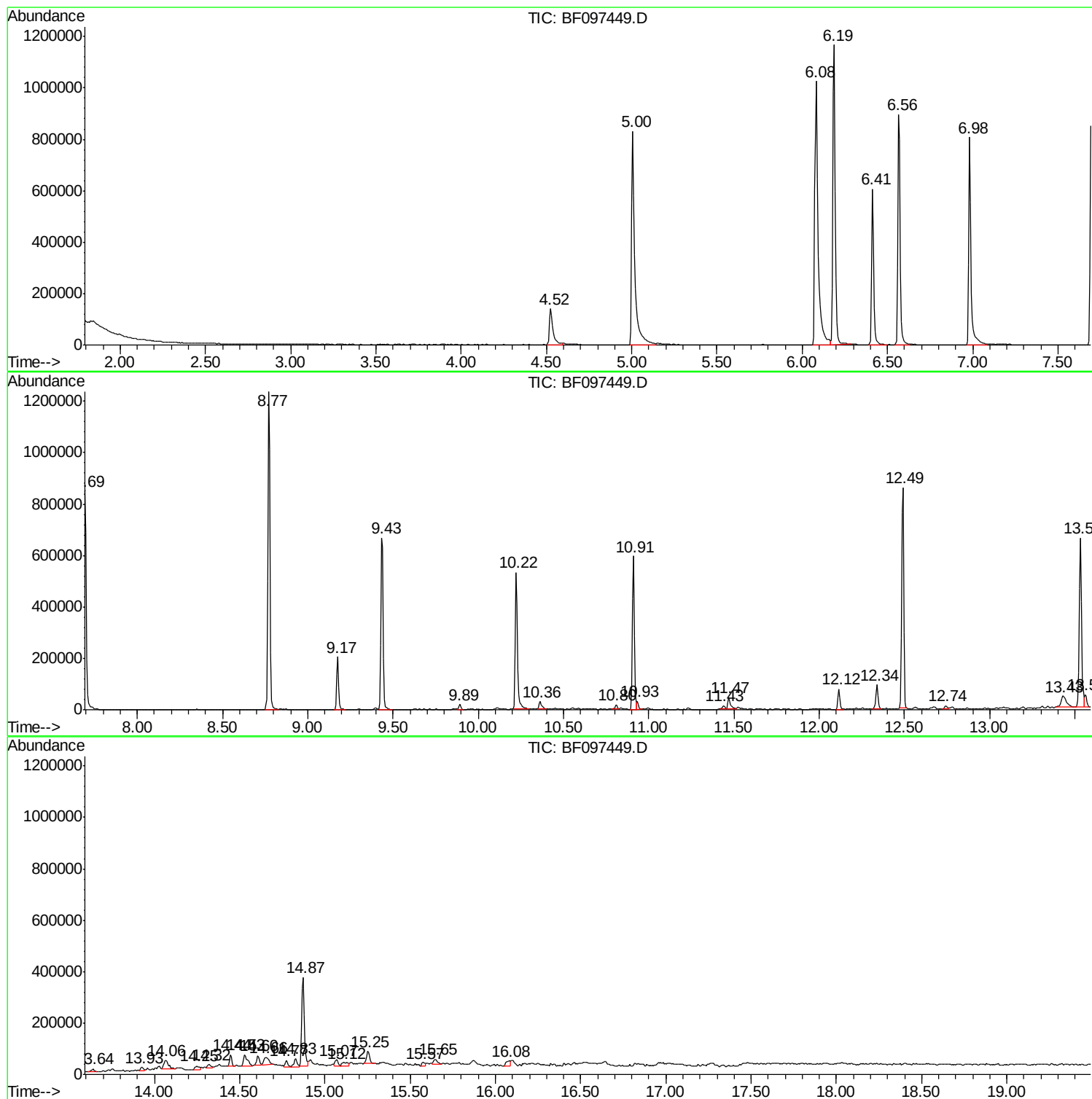
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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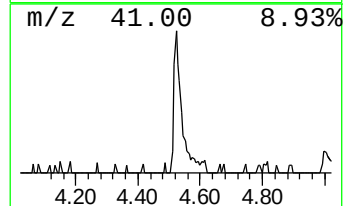
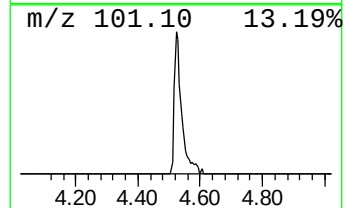
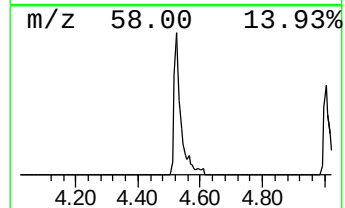
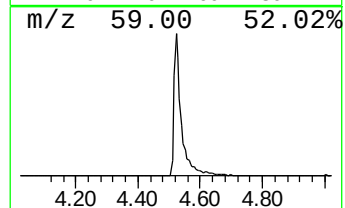
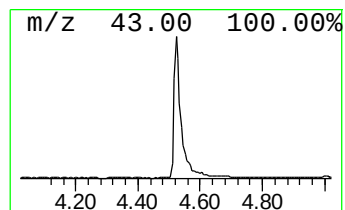
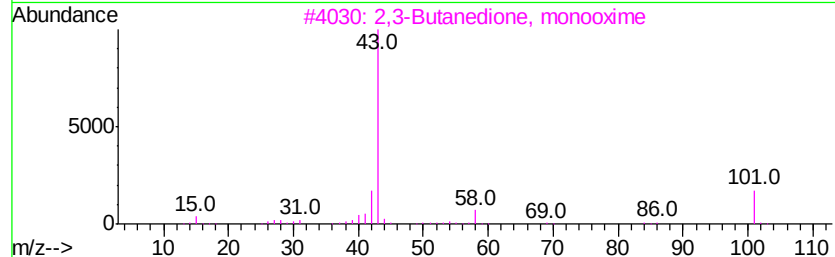
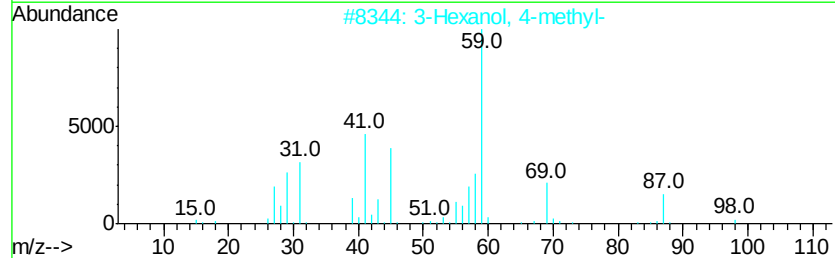
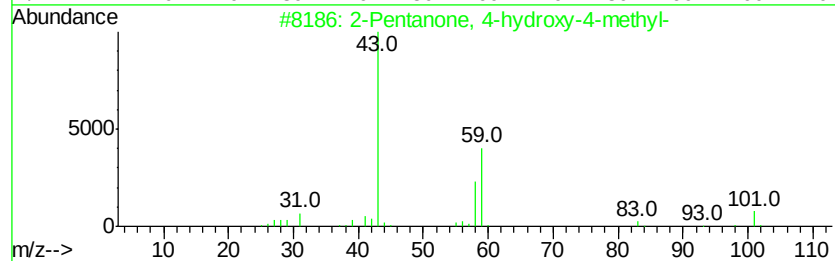
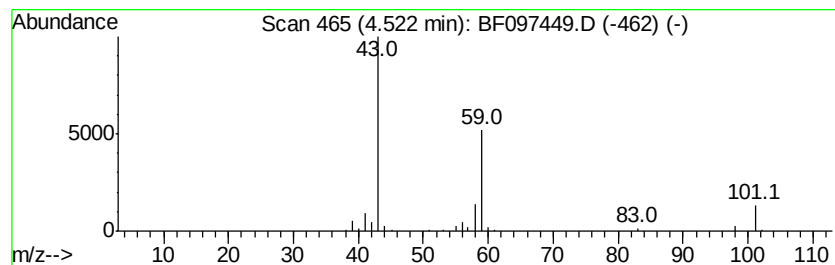
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	7.82 ng	216091	1,4-Dichlorobenzene-d4	6.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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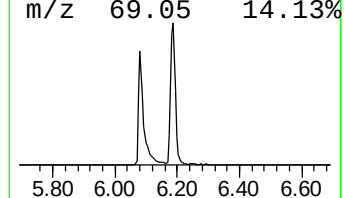
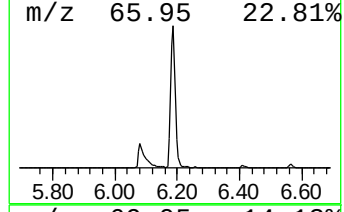
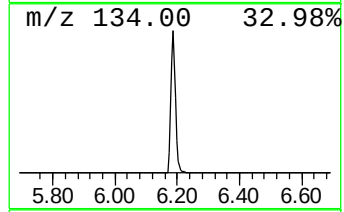
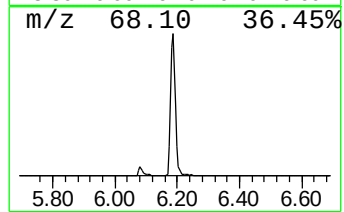
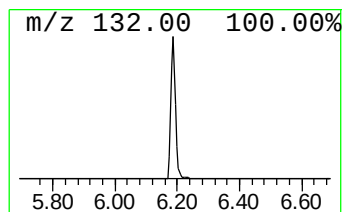
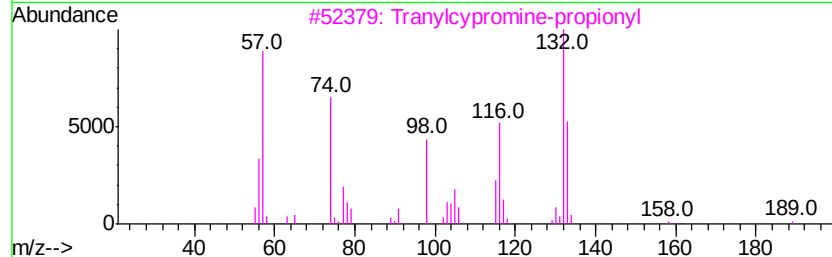
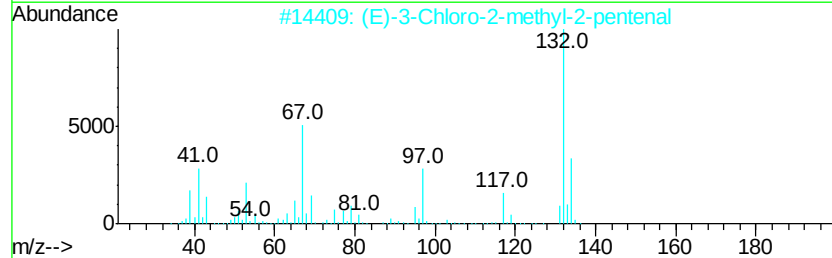
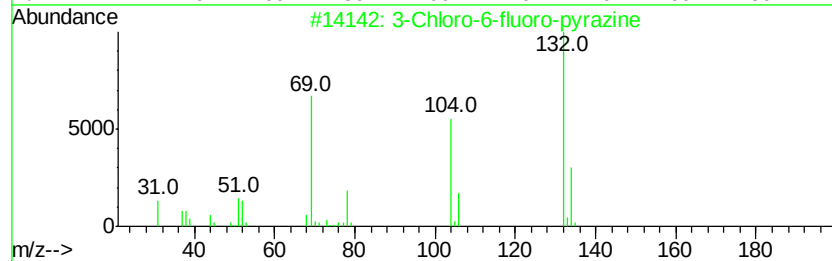
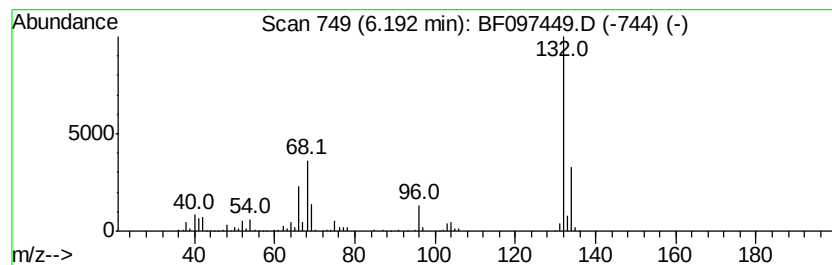
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Peak Number 2 unknown6.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.19	43.77 ng	1209940	1,4-Dichlorobenzene-d4	6.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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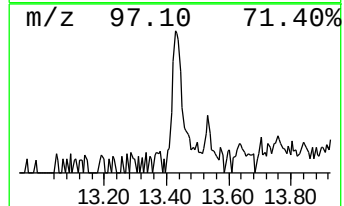
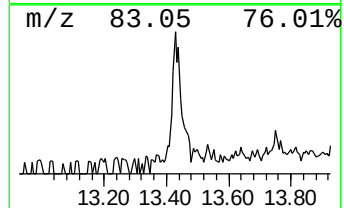
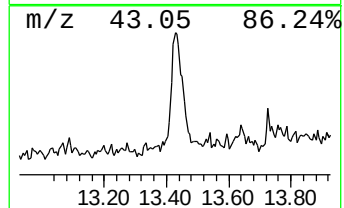
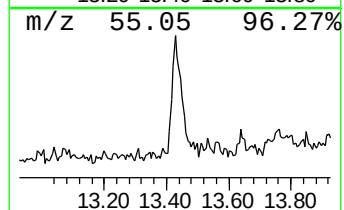
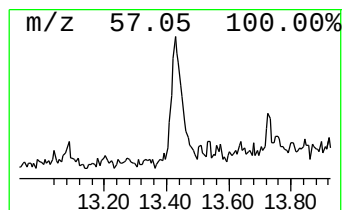
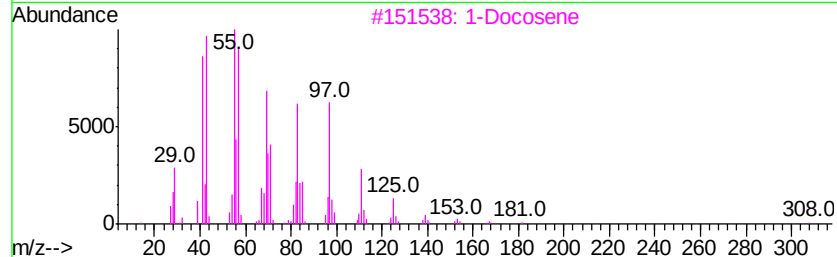
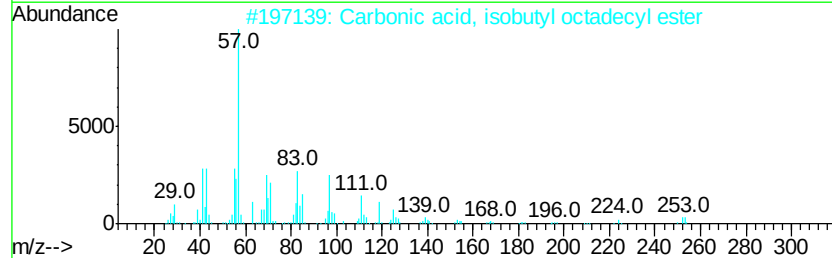
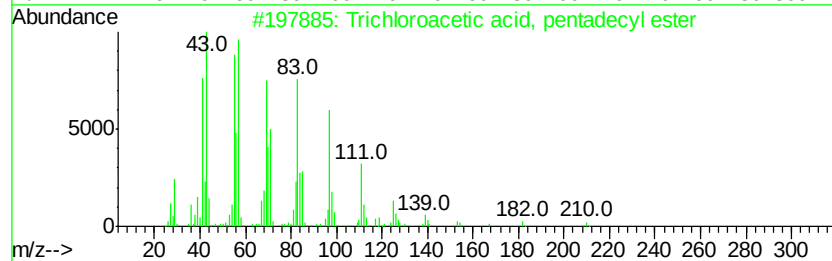
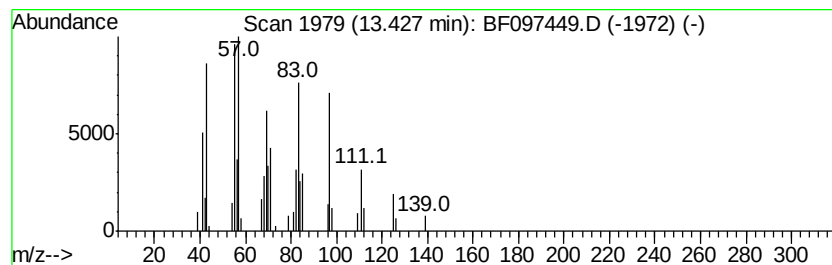
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	3.24 ng	104764	Chrysene-d12	13.53

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
2		Carbonic acid, isobutyl octadecyl...	370	C23H46O3	1000314-61-5	90
3		1-Docosene	308	C22H44	001599-67-3	87
4		1-Hexadecanol	242	C16H34O	036653-82-4	81
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	72



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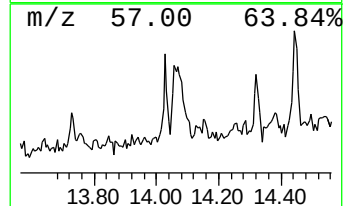
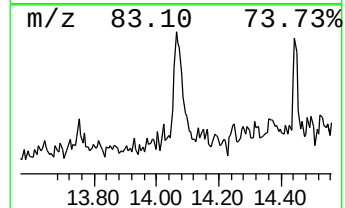
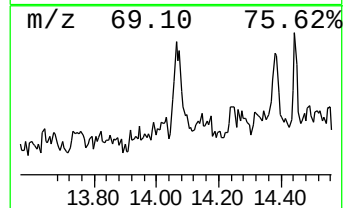
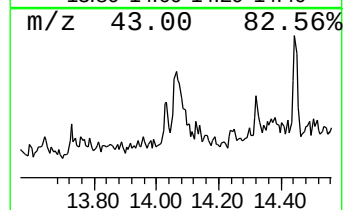
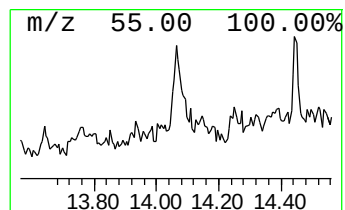
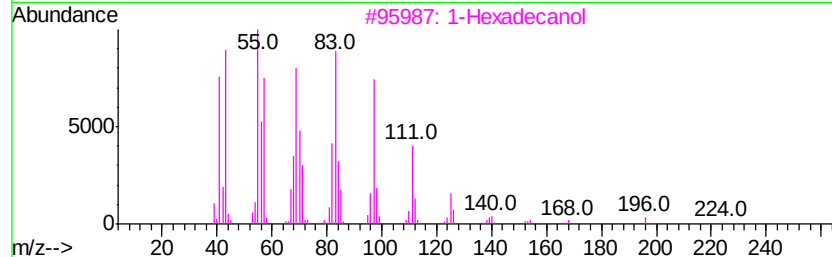
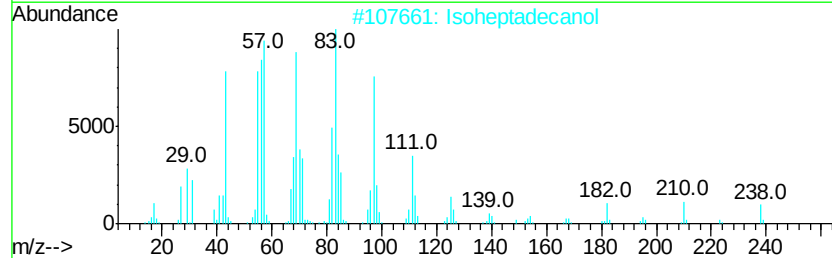
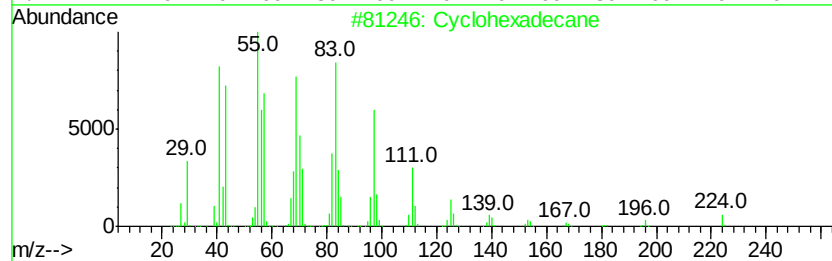
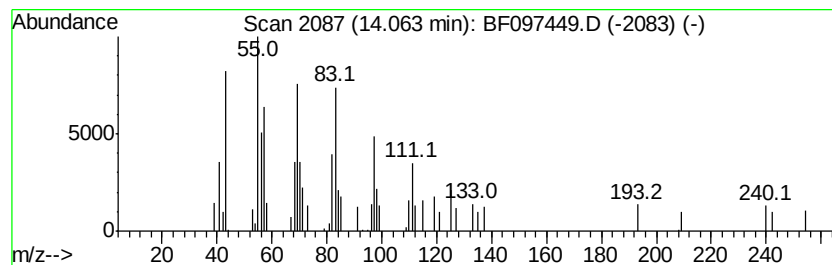
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.06	2.02 ng	65203	Chrysene-d12		13.53
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	83
2	Isoheptadecanol	256	C17H36O	057289-07-3	83
3	1-Hexadecanol	242	C16H34O	036653-82-4	83
4	n-Pentadecanol	228	C15H32O	000629-76-5	80
5	Cyclopentadecane	210	C15H30	000295-48-7	80



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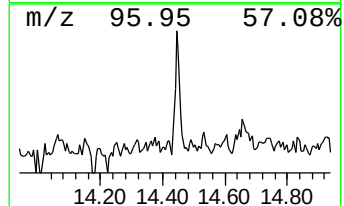
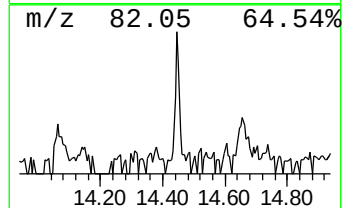
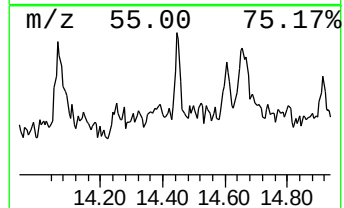
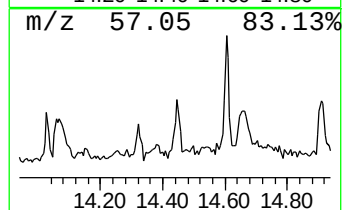
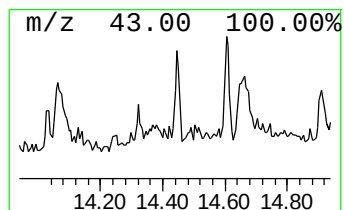
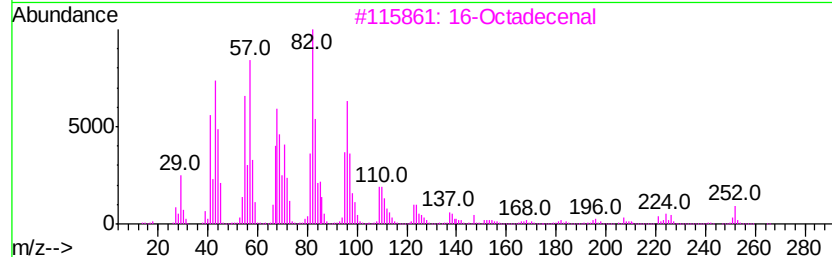
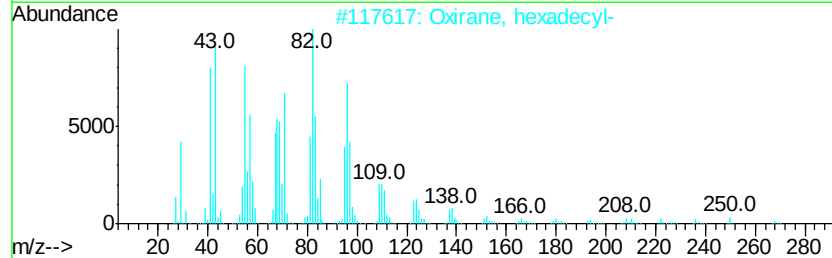
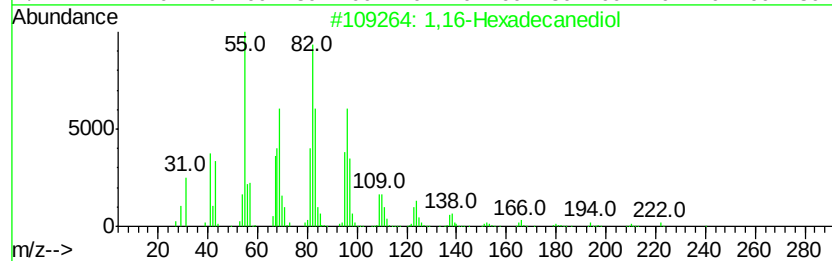
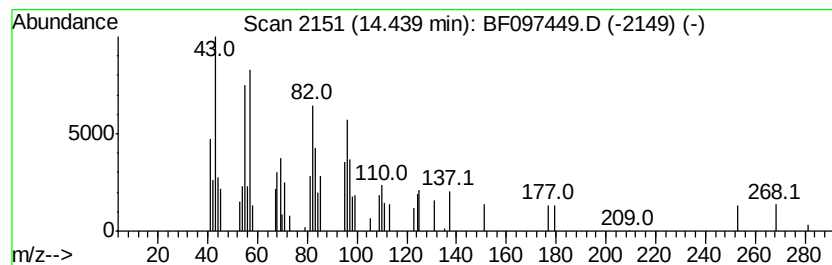
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Peak Number 7 1,16-Hexadecanediol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.44	2.48 ng	47561	Perylene-d12	14.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	80
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
3	16-Octadecenal	266	C18H34O	056554-87-1	74
4	15-Octadecenal	266	C18H34O	056554-93-9	74
5	17-Octadecenal	266	C18H34O	056554-86-0	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080717\
Data File : BF097449.D
Acq On : 8 Aug 2017 00:37
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S2

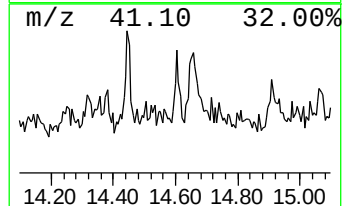
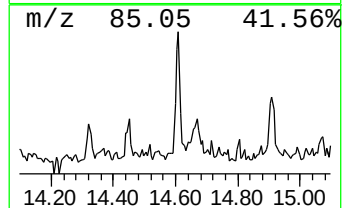
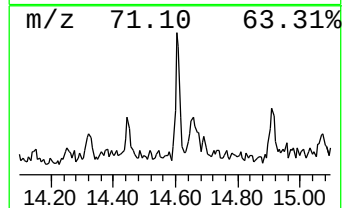
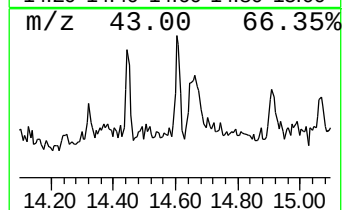
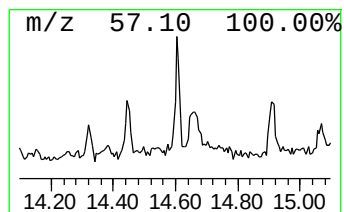
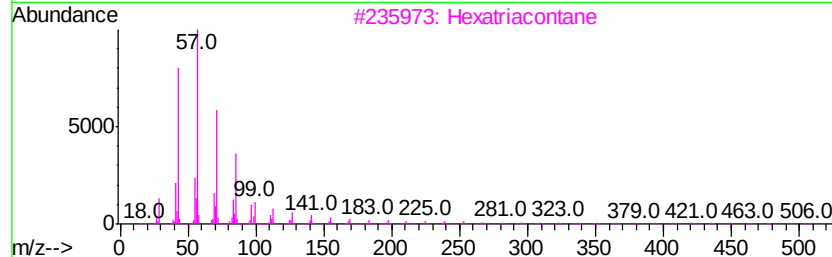
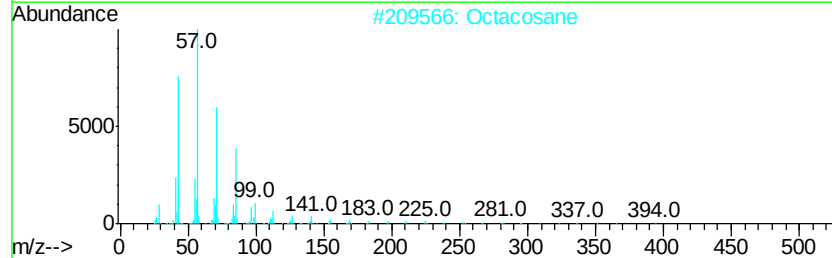
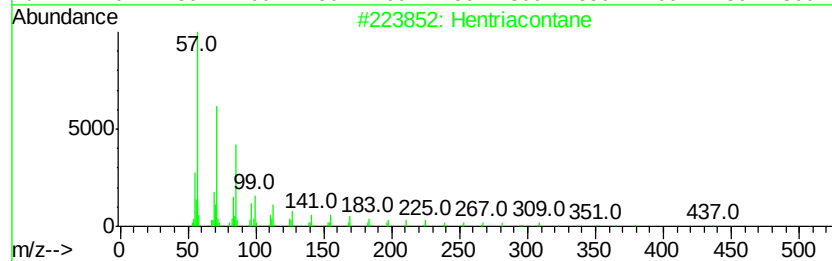
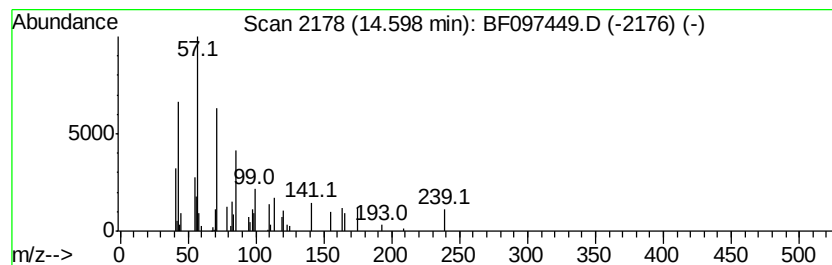
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.42 ng	46339	Perylene-d12	14.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	83
2	Octacosane		394	C28H58	000630-02-4	80
3	Hexatriacontane		507	C36H74	000630-06-8	80
4	Tetratetracontane		619	C44H90	007098-22-8	80
5	Heptacosane		380	C27H56	000593-49-7	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080717\
Data File : BF097449.D
Acq On : 8 Aug 2017 00:37
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

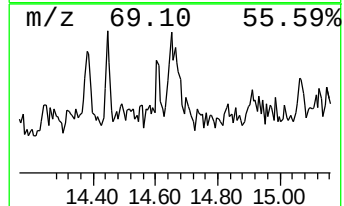
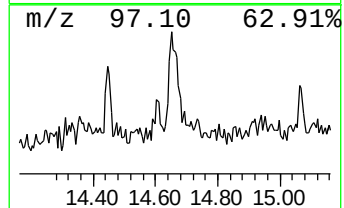
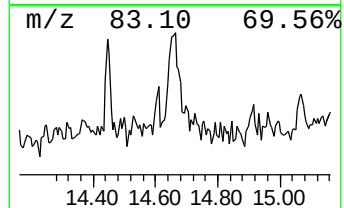
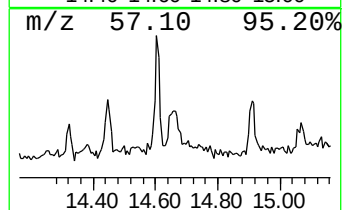
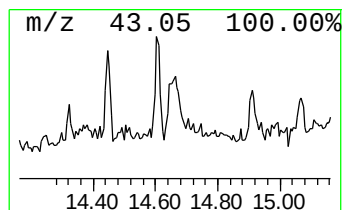
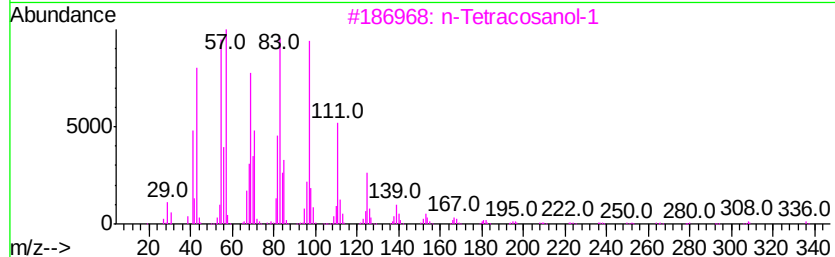
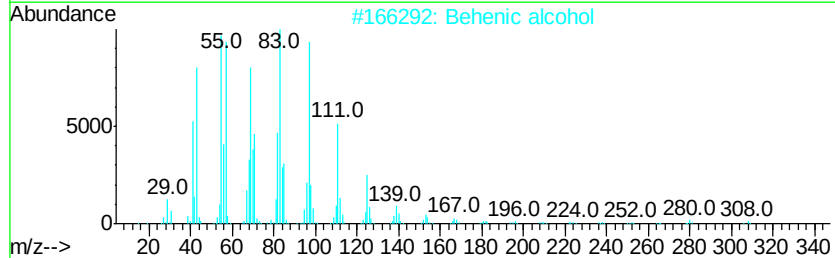
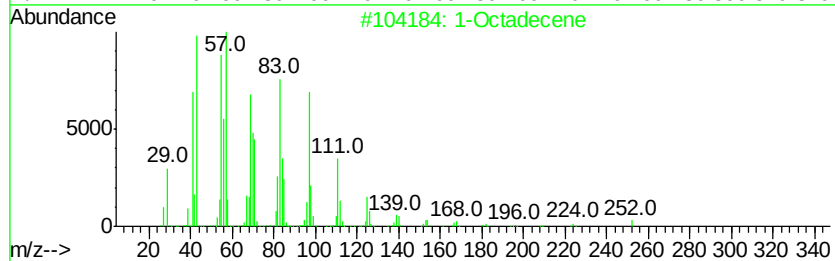
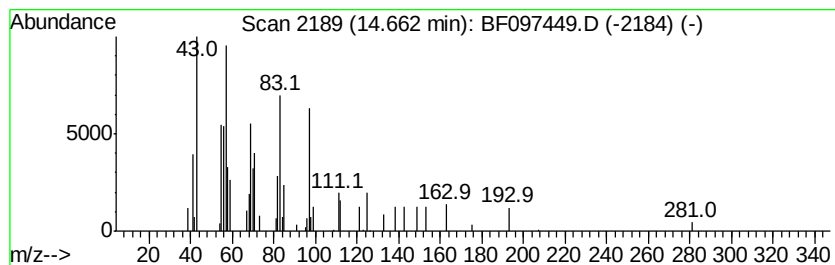
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Octadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.74 ng	52646	Perylene-d12	14.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Octadecene	252 C18H36	000112-88-9	59
2	Behenic alcohol	326 C22H46O	000661-19-8	58
3	n-Tetracosanol-1	354 C24H50O	000506-51-4	58
4	1-Heneicosanol	312 C21H44O	015594-90-8	58
5	n-Nonadecanol-1	284 C19H40O	001454-84-8	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080717\
Data File : BF097449.D
Acq On : 8 Aug 2017 00:37
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S2

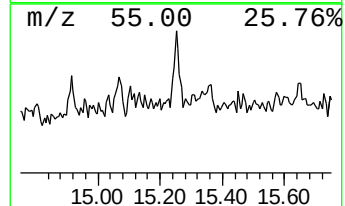
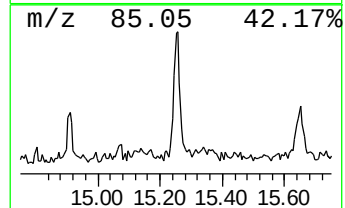
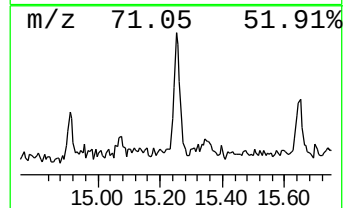
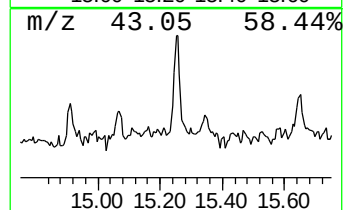
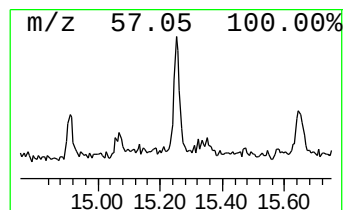
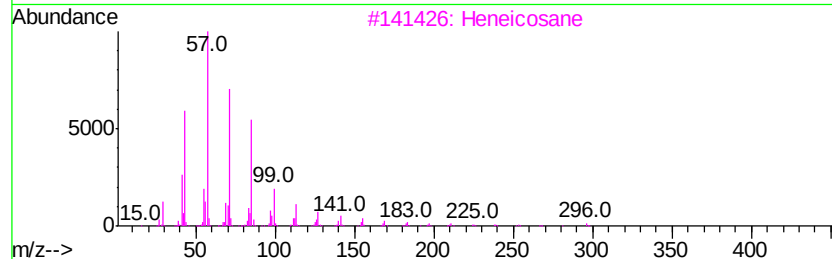
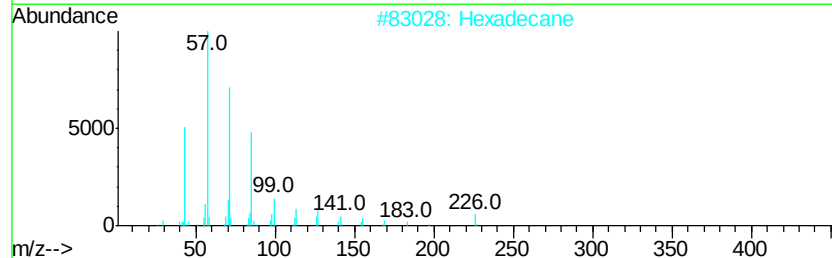
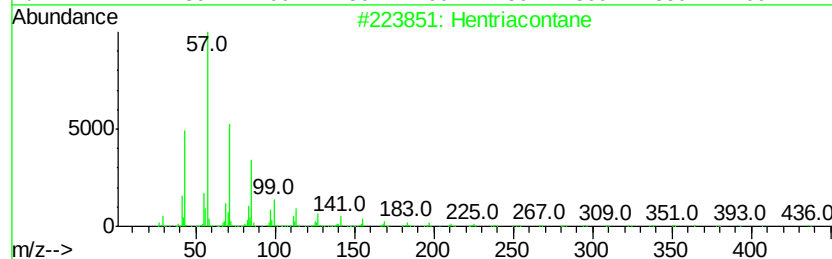
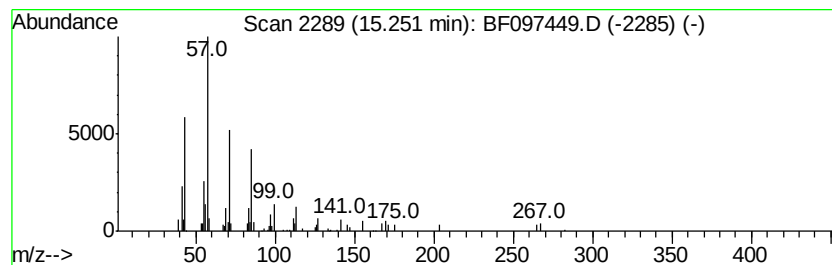
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	3.38 ng	64763	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	83
2		Hexadecane	226	C16H34	000544-76-3	80
3		Heneicosane	296	C21H44	000629-94-7	74
4		Octacosane	394	C28H58	000630-02-4	74
5		Hexacosane	366	C26H54	000630-01-3	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080717\
Data File : BF097449.D
Acq On : 8 Aug 2017 00:37
Operator : SJ/JU
Sample : I4582-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S2

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
2-Pentanone, 4-hy...	4.52	7.8 ng		216091	1	6.41	552809	20.0
unknown6.19	6.19	43.8 ng		1209940	1	6.41	552809	20.0
Trichloroacetic a...	13.43	3.2 ng		104764	5	13.53	646957	20.0
Cyclohexadecane	14.06	2.0 ng		65203	5	13.53	646957	20.0
1,16-Hexadecanediol	14.44	2.5 ng		47561	6	14.87	383687	20.0
Hentriacontane	14.60	2.4 ng		46339	6	14.87	383687	20.0
1-Octadecene	14.66	2.7 ng		52646	6	14.87	383687	20.0
Hexadecane	15.25	3.4 ng		64763	6	14.87	383687	20.0