

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
 Data File : BF088266.D
 Acq On : 22 Jun 2016 23:12
 Operator : UM/SJ
 Sample : H3660-05
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3(0-6)

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-BF060716.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	1.724	10	12	50	rVB	1078595	2233410	100.00%	11.093%
2	4.719	272	274	288	rBV	261047	404354	18.10%	2.008%
3	5.187	313	315	317	rBV	1315681	1550306	69.41%	7.700%
4	5.599	349	351	356	rVB	19014	29224	1.31%	0.145%
5	6.262	407	409	411	rBV	1487761	1546220	69.23%	7.680%
6	6.376	417	419	421	rBV	1320387	1656119	74.15%	8.225%
7	6.604	437	439	441	rBV	428182	450946	20.19%	2.240%
8	6.753	450	452	455	rBV	1327566	1265172	56.65%	6.284%
9	7.176	486	489	491	rBV	1141718	1063417	47.61%	5.282%
10	7.885	549	551	554	rBV	619960	637930	28.56%	3.168%
11	8.970	643	646	648	rBV	2145894	1989155	89.06%	9.879%
12	9.370	679	681	683	rBV	319781	272673	12.21%	1.354%
13	9.633	702	704	707	rBV	745286	679242	30.41%	3.374%
14	9.793	716	718	724	rBV	22017	40270	1.80%	0.200%
15	10.422	771	773	776	rBV	987148	946549	42.38%	4.701%
16	10.548	782	784	791	rVB	26391	34656	1.55%	0.172%
17	10.993	821	823	825	rBV	32744	34294	1.54%	0.170%
18	11.108	832	833	835	rBV	421839	574781	25.74%	2.855%
19	11.142	835	836	838	rVV	53696	46688	2.09%	0.232%
20	11.188	838	840	843	rVB2	10477	22920	1.03%	0.114%
21	11.416	858	860	865	rVB	25580	36491	1.63%	0.181%
22	11.668	879	882	885	rBV	32734	64859	2.90%	0.322%
23	12.319	937	939	942	rBV3	106940	116194	5.20%	0.577%
24	12.548	954	959	963	rBV	117476	126211	5.65%	0.627%
25	12.697	969	972	974	rBV	1495198	1383910	61.96%	6.873%
26	12.937	990	993	995	rBV2	13497	24563	1.10%	0.122%
27	13.279	1020	1023	1026	rBV3	7456	22576	1.01%	0.112%
28	13.519	1040	1044	1046	rBV4	13985	33594	1.50%	0.167%
29	13.611	1050	1052	1060	rBV3	71801	150637	6.74%	0.748%
30	13.737	1061	1063	1065	rBV	407676	558290	25.00%	2.773%
31	13.919	1076	1079	1080	rBV2	14316	23957	1.07%	0.119%
32	14.251	1103	1108	1112	rBV4	43303	140031	6.27%	0.695%
33	14.582	1135	1137	1138	rVB	22713	27734	1.24%	0.138%
34	14.640	1140	1142	1145	rVB	142881	159542	7.14%	0.792%

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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

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Peak separation: 5

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35	14.742	1150	1151	1155	rVV	62007	114026	5.11%	0.566%
36	14.811	1155	1157	1158	rVV	82270	87402	3.91%	0.434%
37	14.845	1158	1160	1165	rVV2	79230	177213	7.93%	0.880%
38	15.005	1172	1174	1177	rBV	38215	48500	2.17%	0.241%
39	15.062	1177	1179	1181	rBV	41744	57413	2.57%	0.285%
40	15.108	1181	1183	1189	rVB	377393	474326	21.24%	2.356%
41	15.302	1197	1200	1203	rVB3	54428	96539	4.32%	0.479%
42	15.497	1214	1217	1219	rBV	108292	165923	7.43%	0.824%
43	16.148	1271	1274	1278	rVB	70098	128826	5.77%	0.640%
44	16.400	1293	1296	1299	rVB2	55564	109069	4.88%	0.542%
45	16.548	1307	1309	1310	rBV	15637	26796	1.20%	0.133%
46	16.823	1327	1333	1339	rVB2	28101	120764	5.41%	0.600%
47	17.634	1401	1404	1410	rVB3	39486	111586	5.00%	0.554%
48	19.154	1533	1537	1546	rVB5	20094	68971	3.09%	0.343%

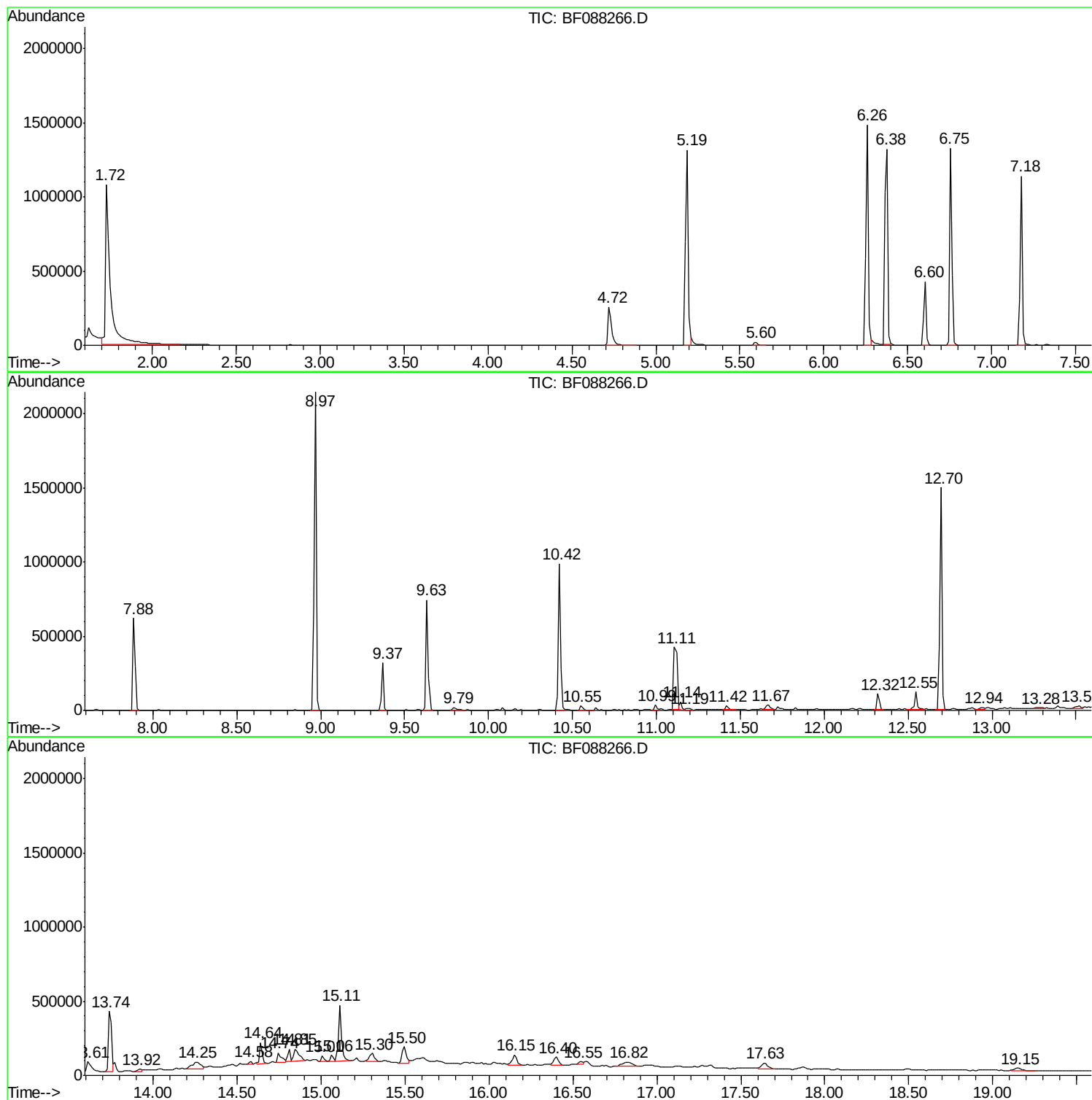
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : H3660-05
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
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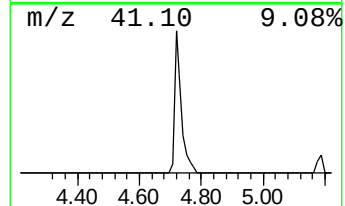
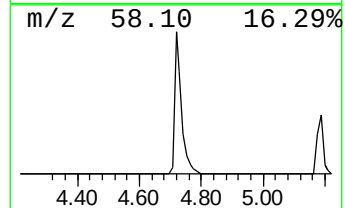
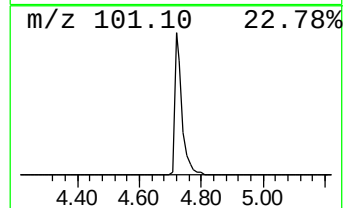
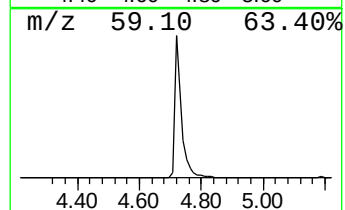
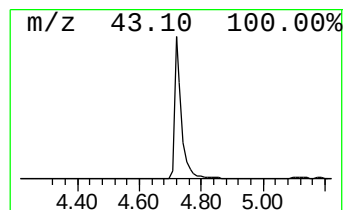
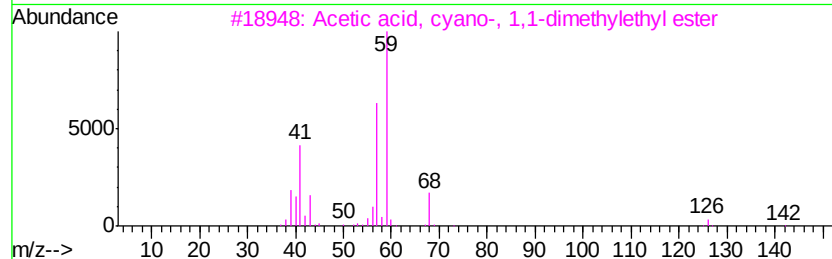
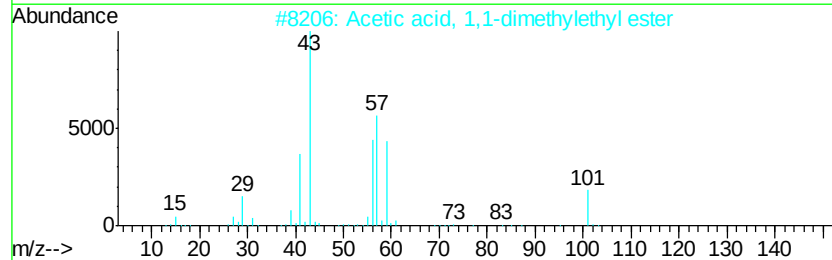
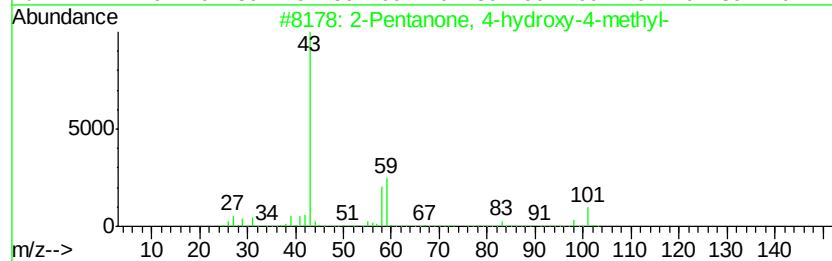
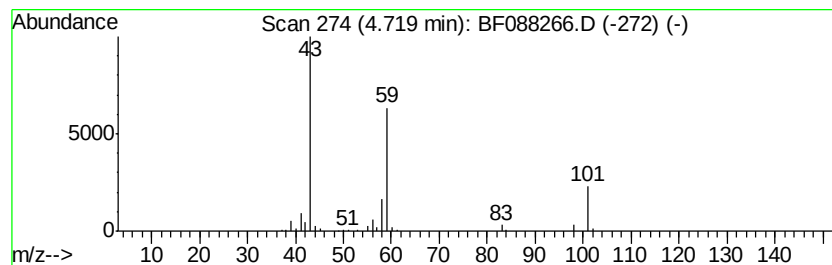
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	17.93 ng	404354	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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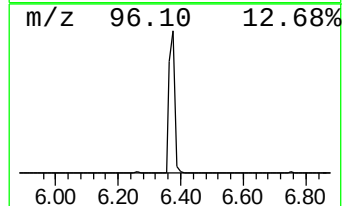
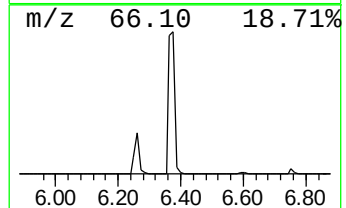
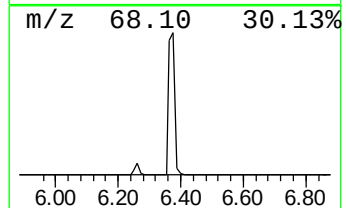
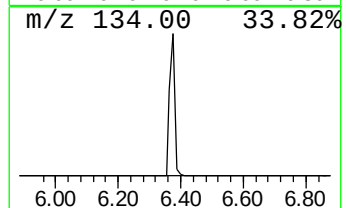
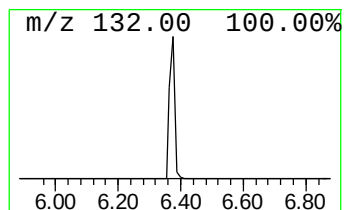
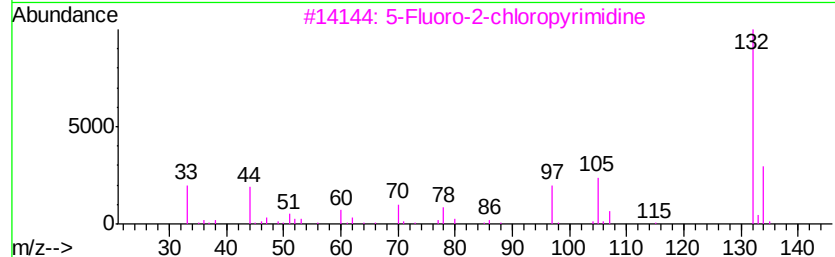
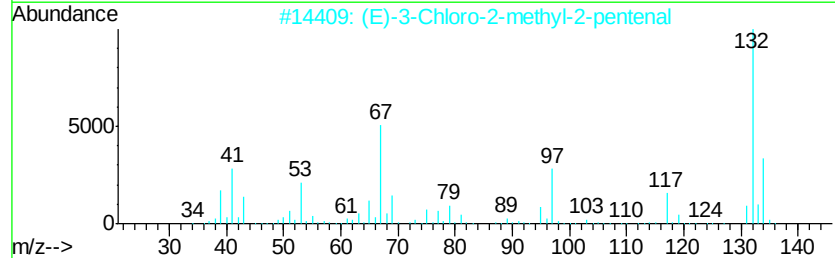
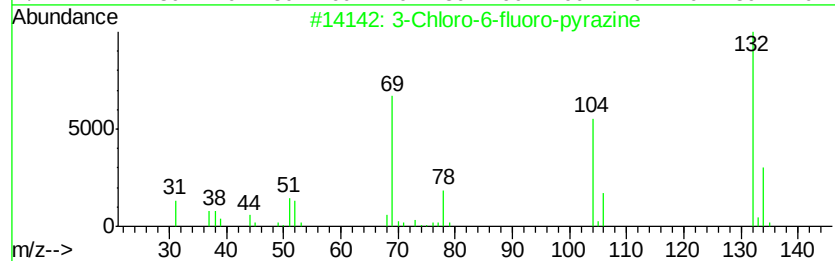
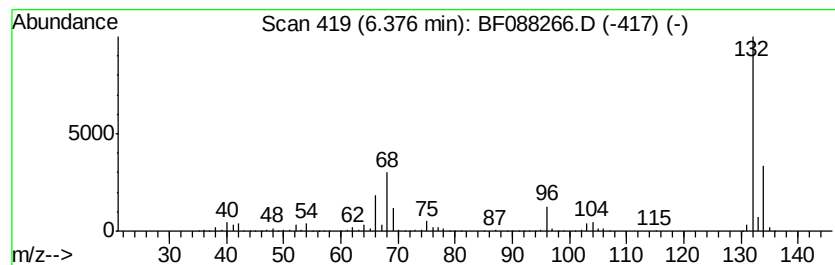
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Peak Number 3 3-Chloro-6-fluoro-pyrazine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	73.45 ng	1656120	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	52
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	33
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		Xenon	132	Xe	007440-63-3	9



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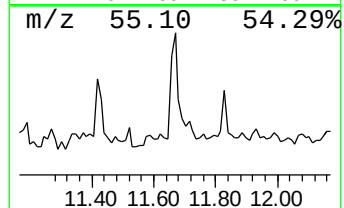
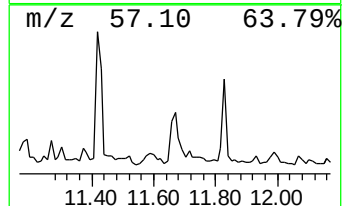
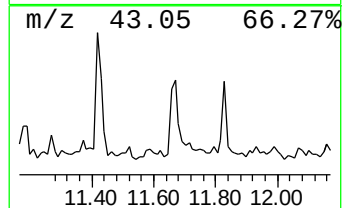
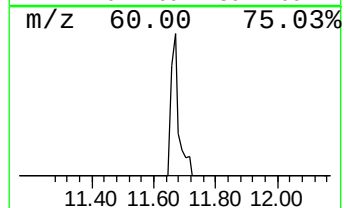
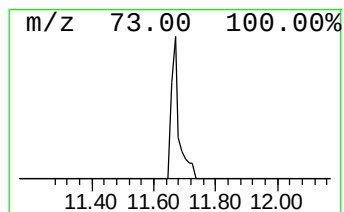
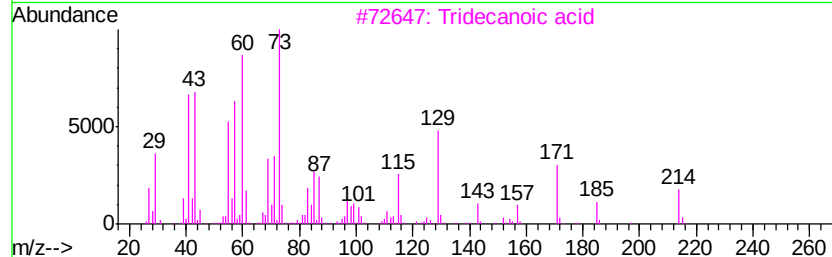
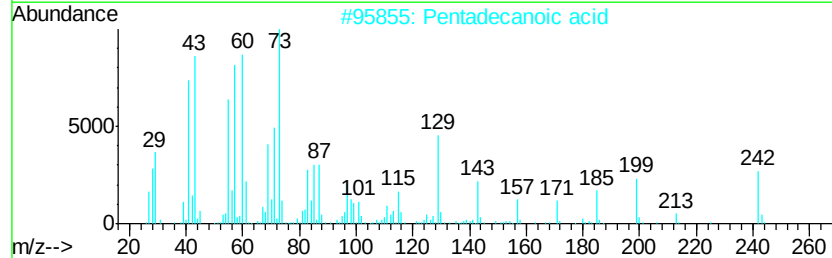
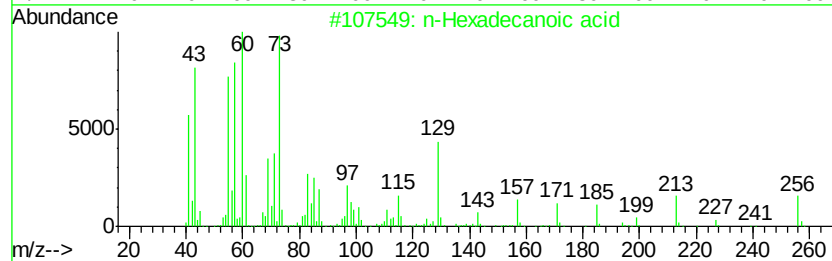
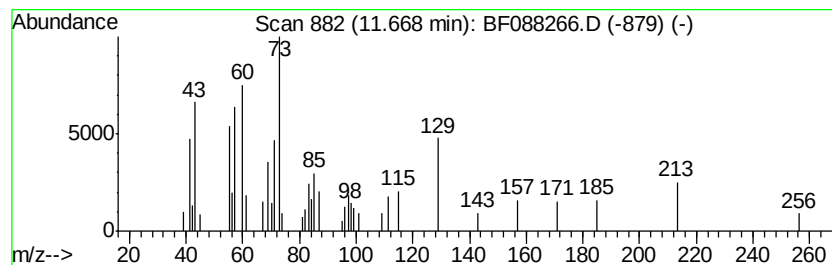
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	2.26 ng	64859	Phenanthrene-d10	11.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	74
4		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



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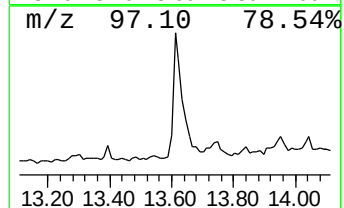
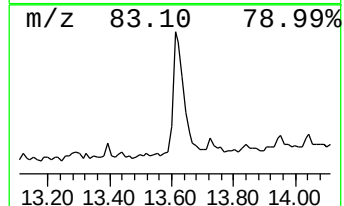
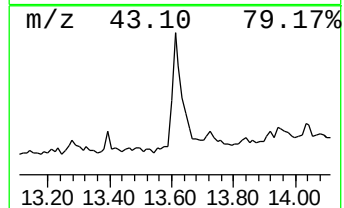
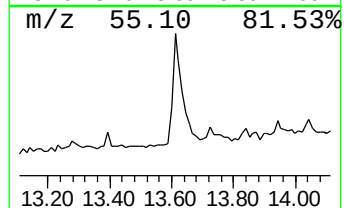
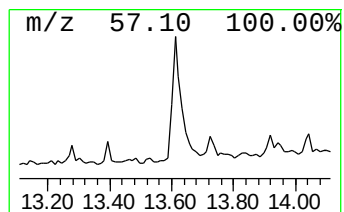
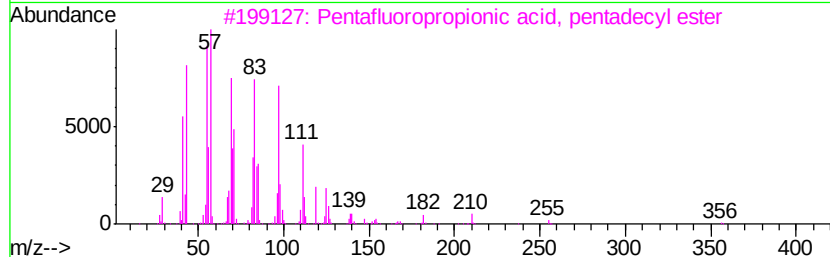
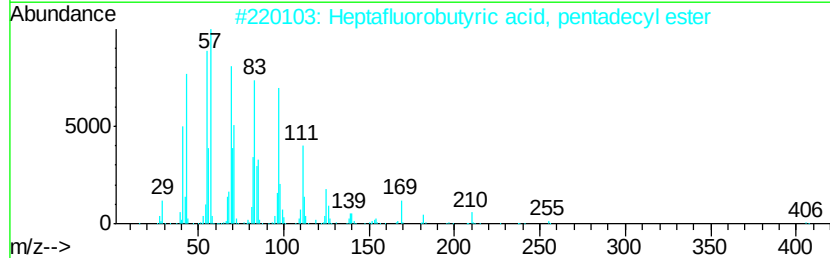
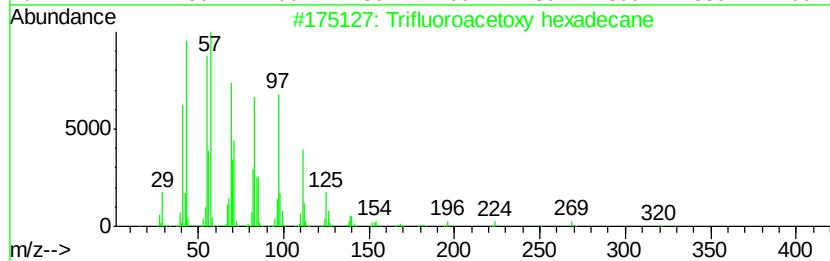
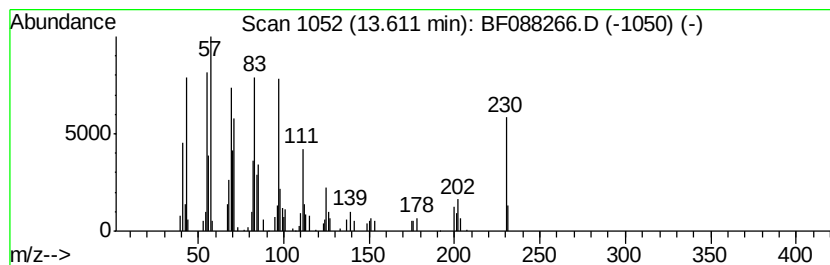
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	5.40 ng	150637	Chrysene-d12	13.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93



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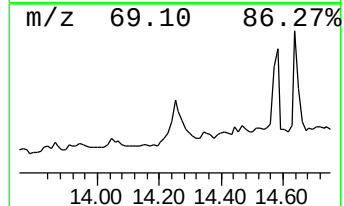
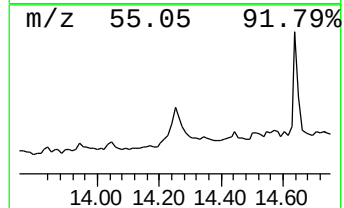
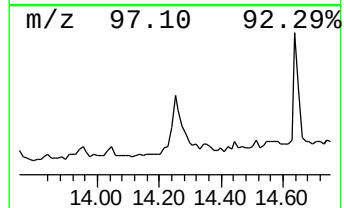
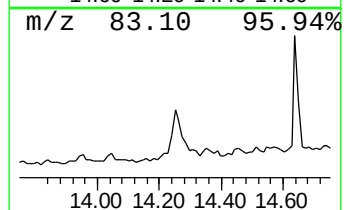
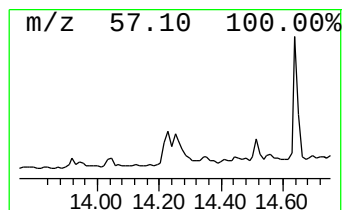
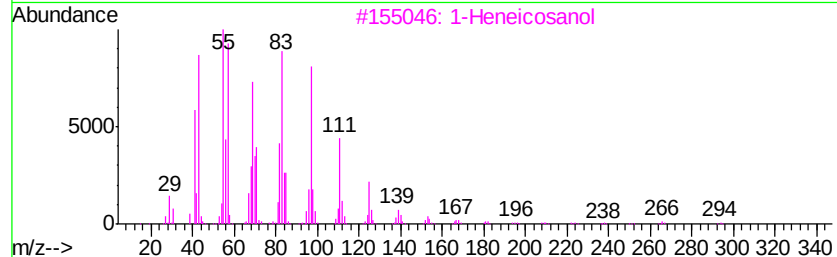
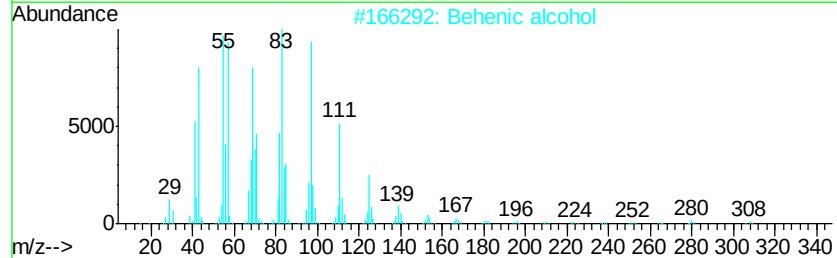
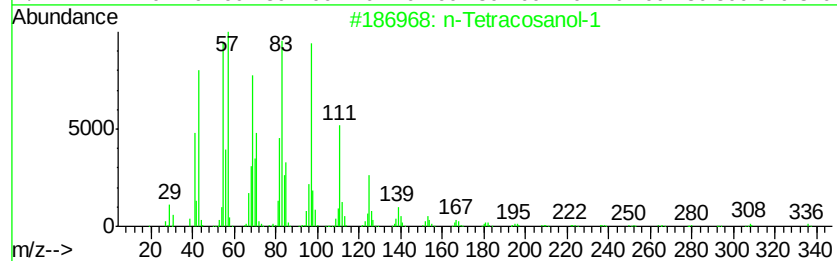
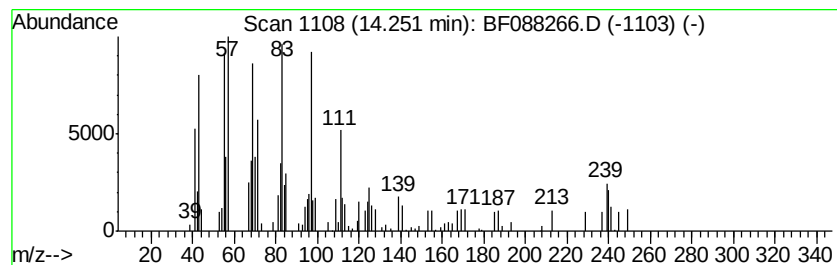
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Tetracosanol-1 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.25	5.02 ng	140031	Chrysene-d12	13.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	81
2	Behenic alcohol	326	C22H46O	000661-19-8	81
3	1-Heneicosanol	312	C21H44O	015594-90-8	81
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	81
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	74



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
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Acq On : 22 Jun 2016 23:12
Operator : UM/SJ
Sample : H3660-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

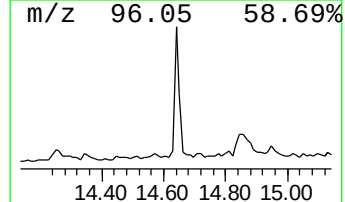
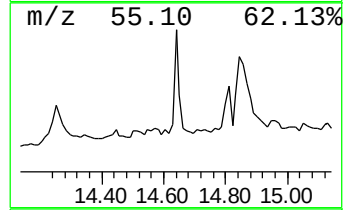
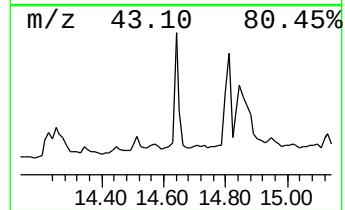
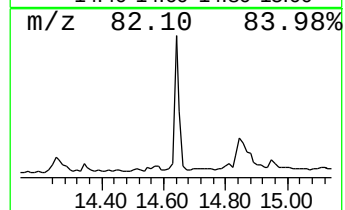
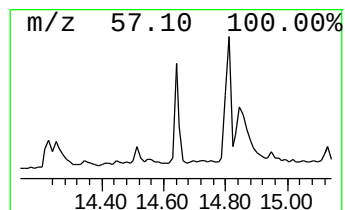
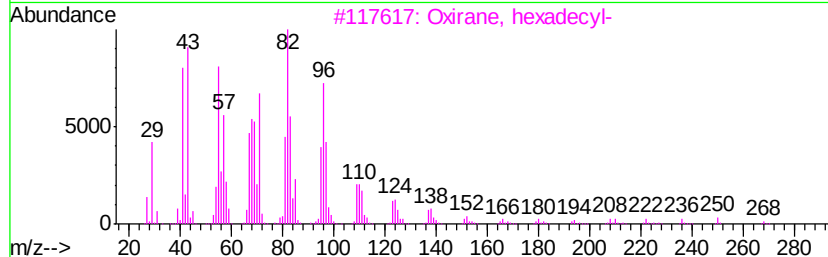
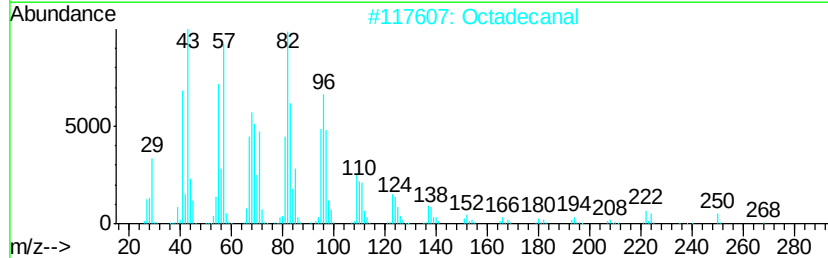
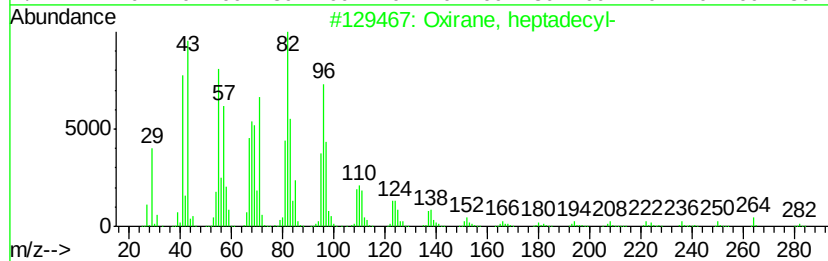
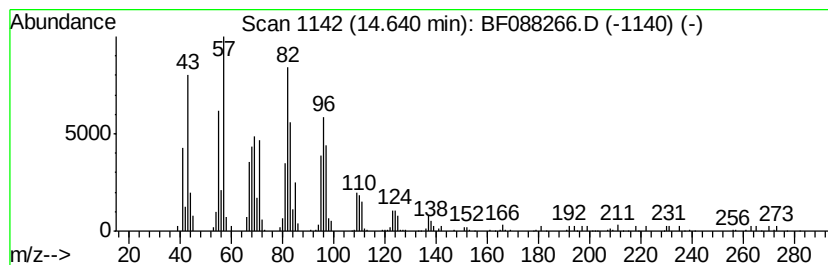
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, heptadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.64	6.73 ng	159542	Perylene-d12	15.11	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
2	Octadecanal	268	C18H36O	000638-66-4	94
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4	16-Octadecenal	266	C18H34O	056554-87-1	91
5	Heptadecanal	254	C17H34O	1000376-70-0	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
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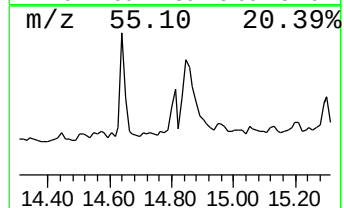
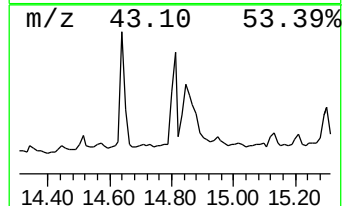
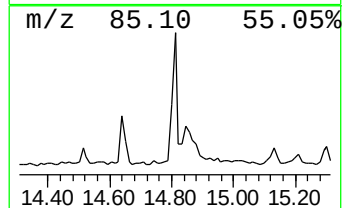
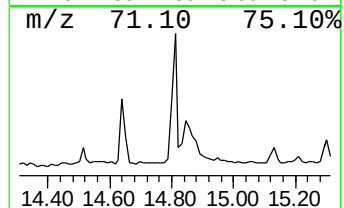
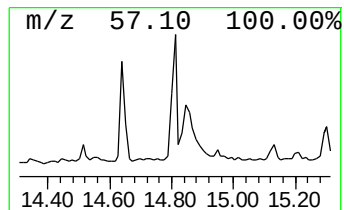
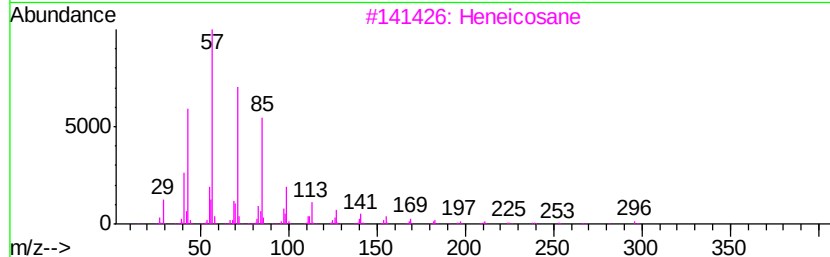
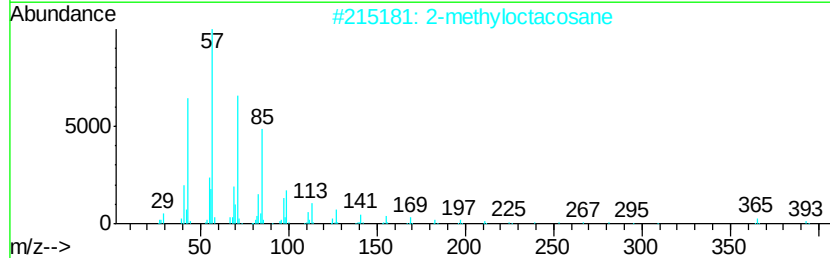
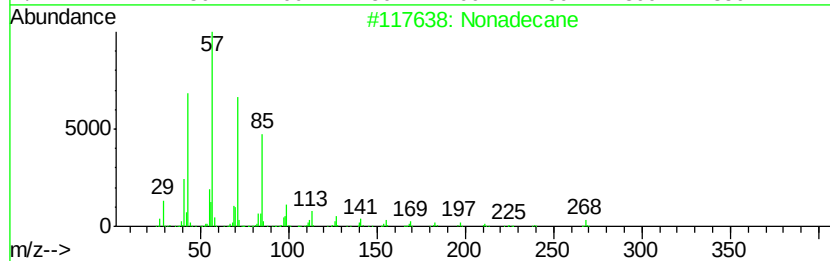
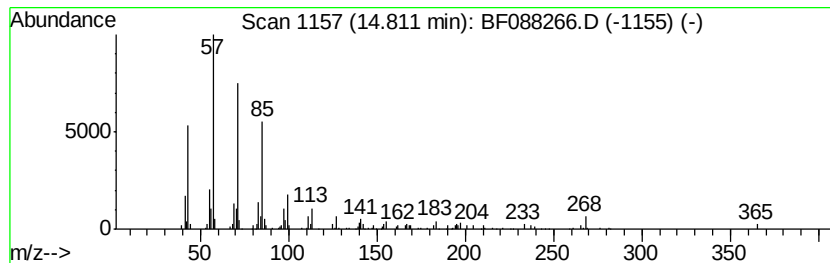
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.81	3.69 ng	87402	Perylene-d12	15.11	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	Eicosane	282	C20H42	000112-95-8	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062216\
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Operator : UM/SJ
Sample : H3660-05
Misc :
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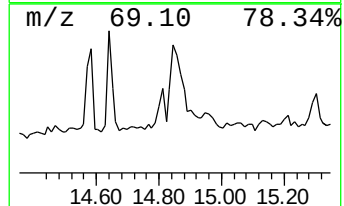
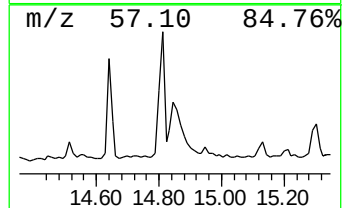
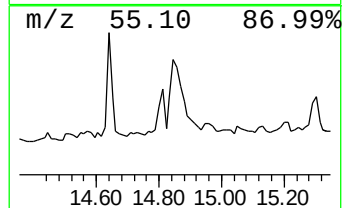
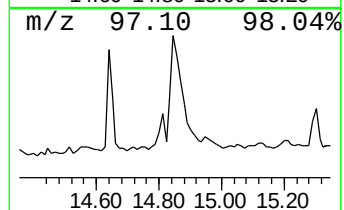
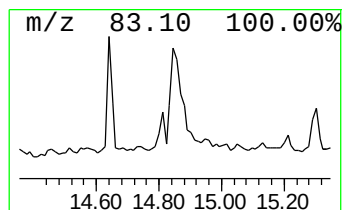
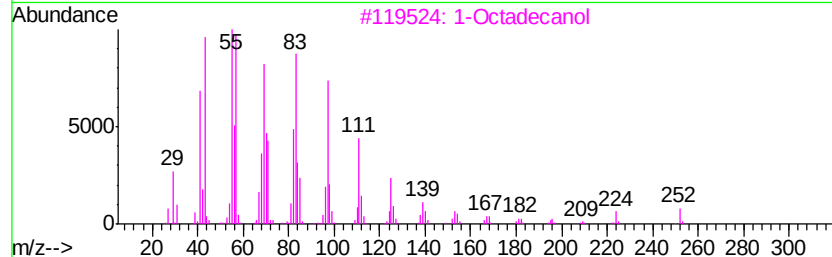
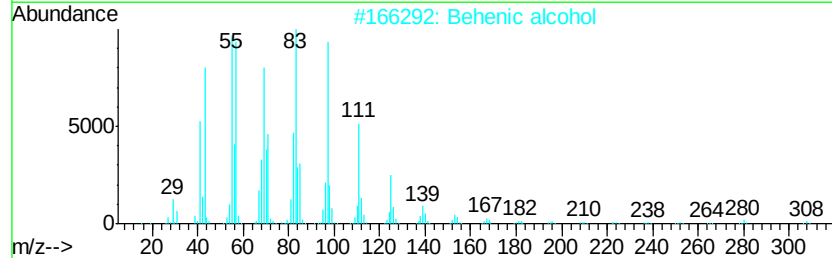
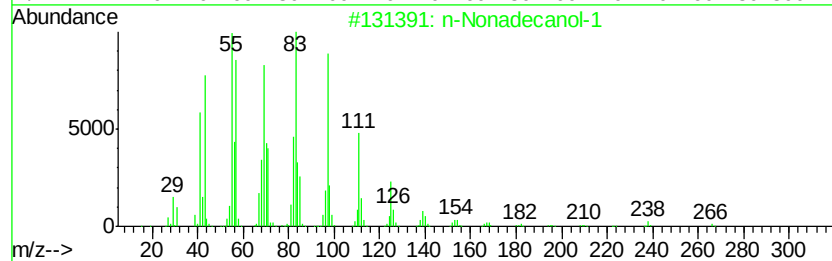
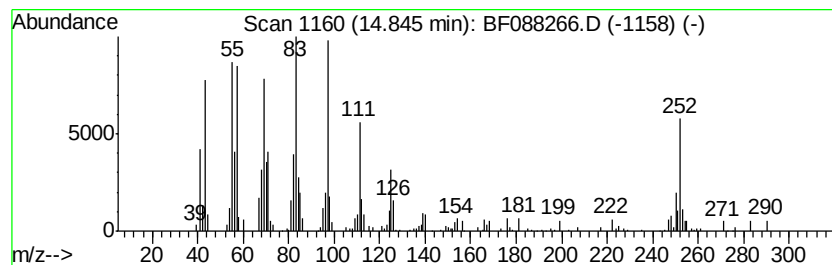
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.85	7.47 ng	177213	Perylene-d12		15.11
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2	Behenic alcohol	326	C22H46O	000661-19-8	89
3	1-Octadecanol	270	C18H38O	000112-92-5	87
4	3-Octadecene, (E)-	252	C18H36	007206-19-1	86
5	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088266.D
Acq On : 22 Jun 2016 23:12
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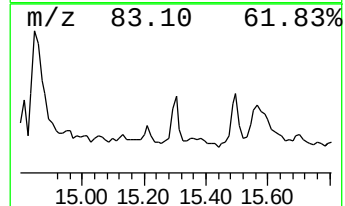
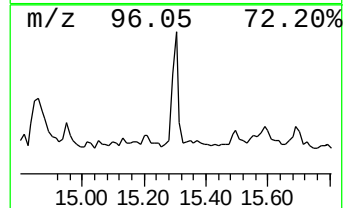
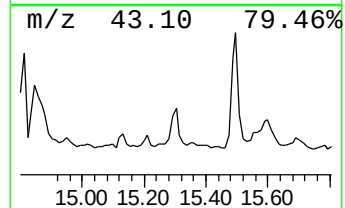
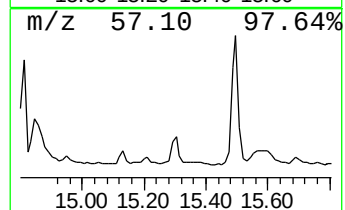
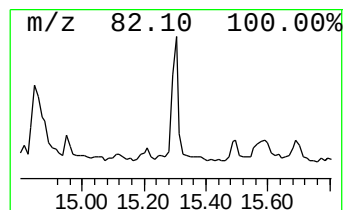
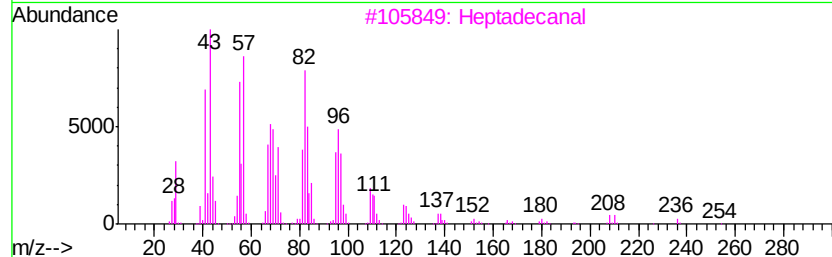
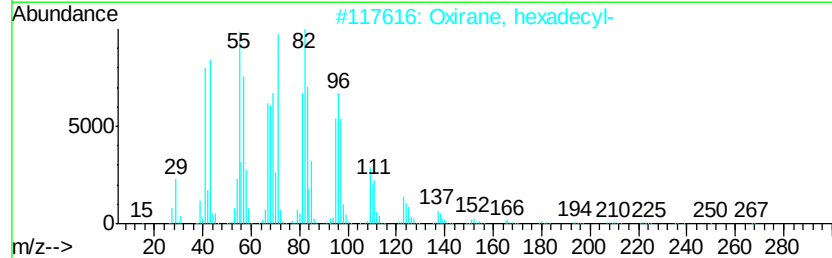
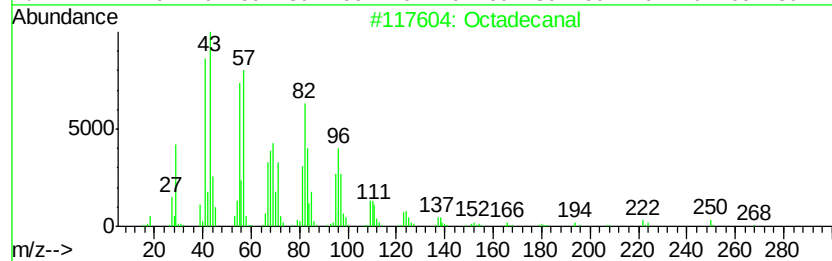
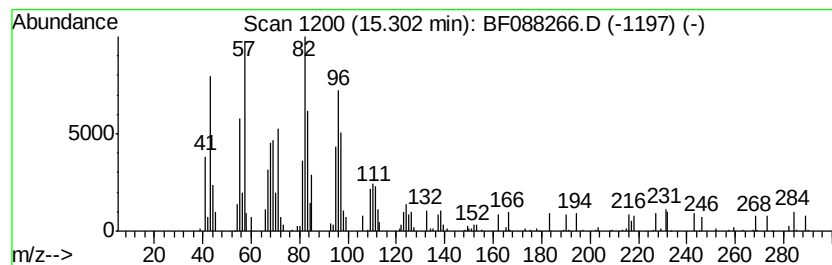
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanal Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	4.07 ng	96539	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	87
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
3		Heptadecanal	254	C17H34O	1000376-70-0	86
4		1,19-Eicosadiene	278	C20H38	014811-95-1	83
5		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088266.D
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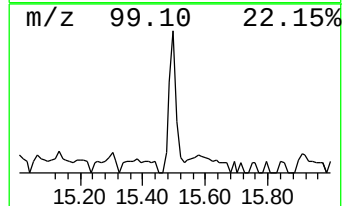
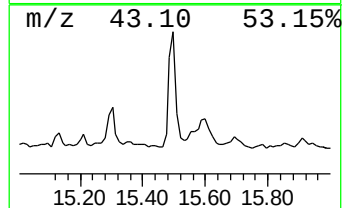
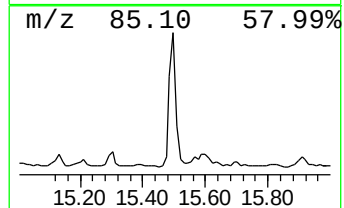
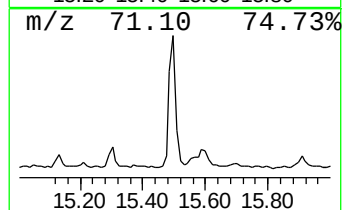
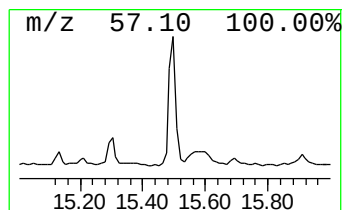
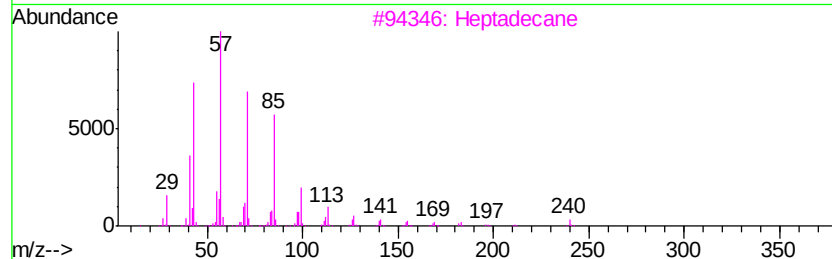
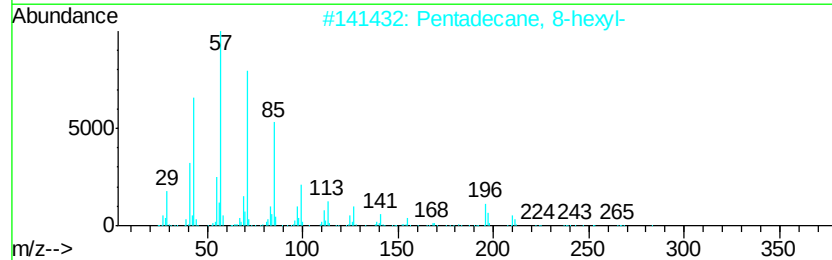
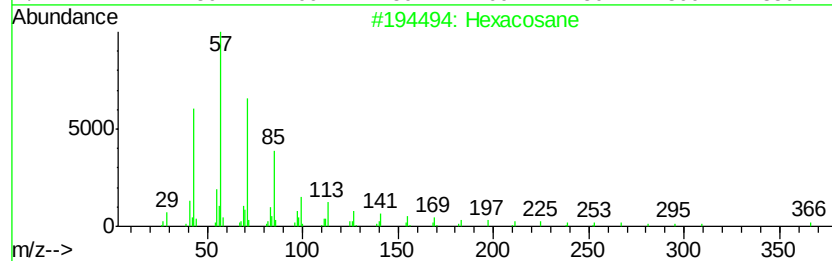
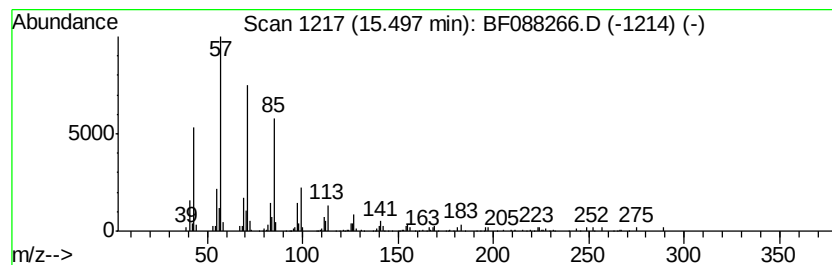
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.50	7.00 ng	165923	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
3		Heptadecane	240	C17H36	000629-78-7	87
4		Tridecane, 6-propyl-	226	C16H34	055045-10-8	83
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
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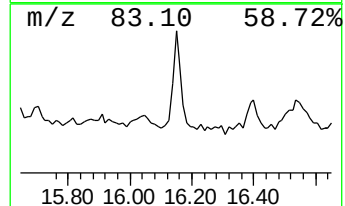
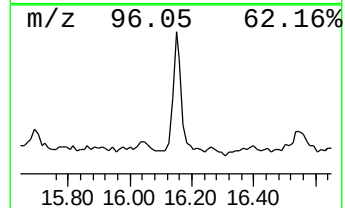
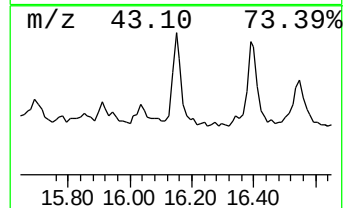
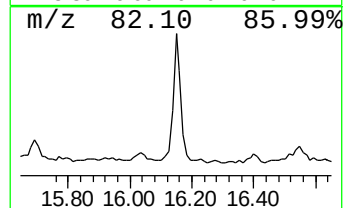
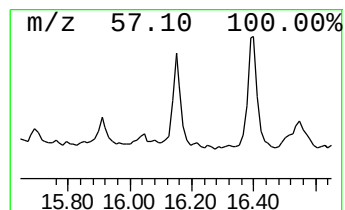
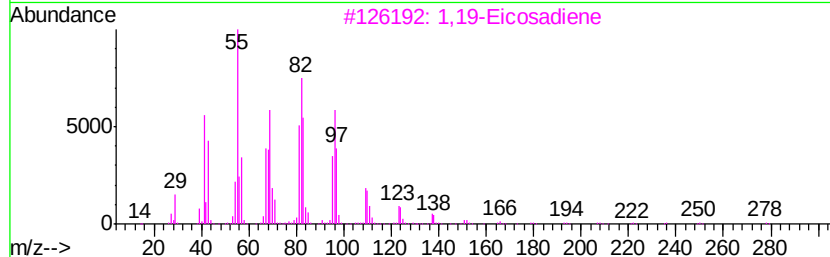
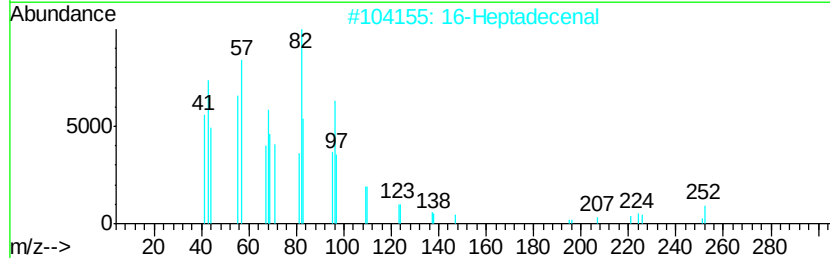
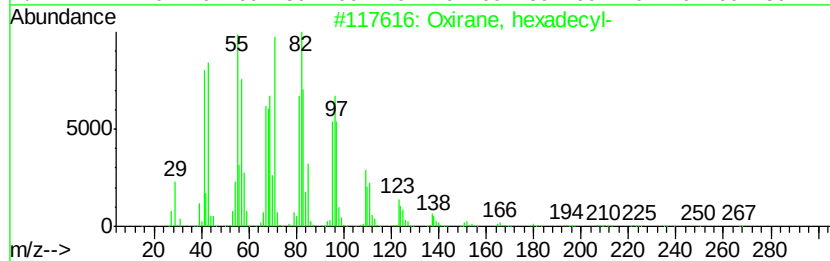
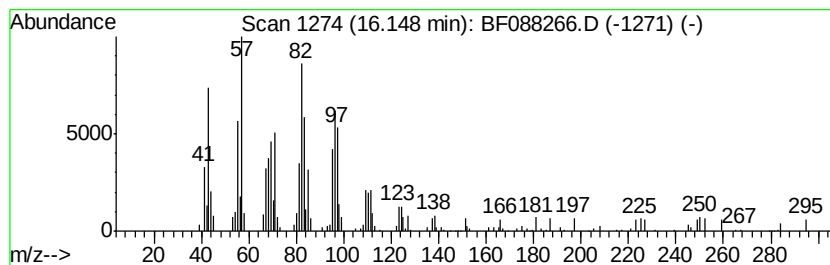
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	5.43 ng	128826	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2		16-Heptadecenal	252	C17H32O	1000144-57-9	90
3		1,19-Eicosadiene	278	C20H38	014811-95-1	81
4		18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	74
5		trans-2-Dodecen-1-ol, trifluoroa...	280	C14H23F3O2	1000352-26-2	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062216\
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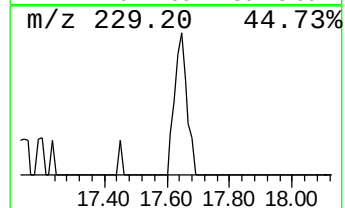
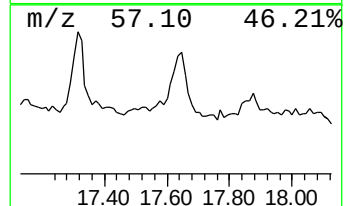
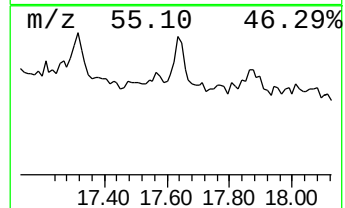
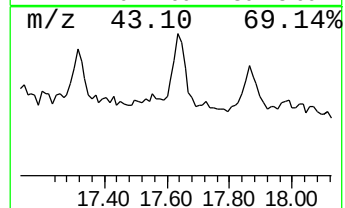
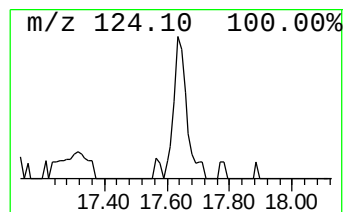
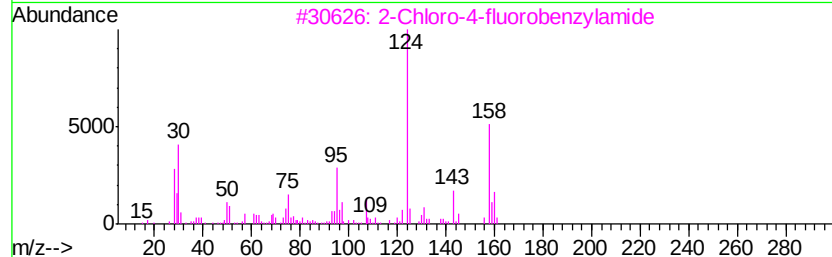
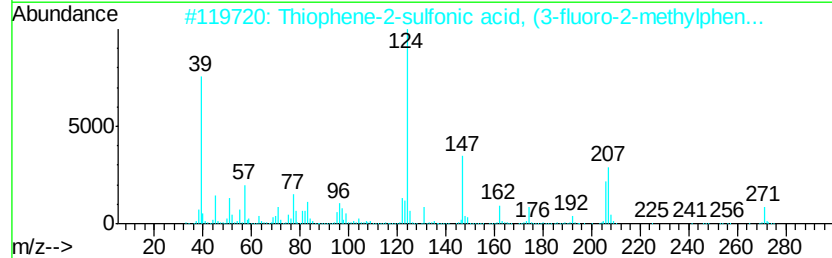
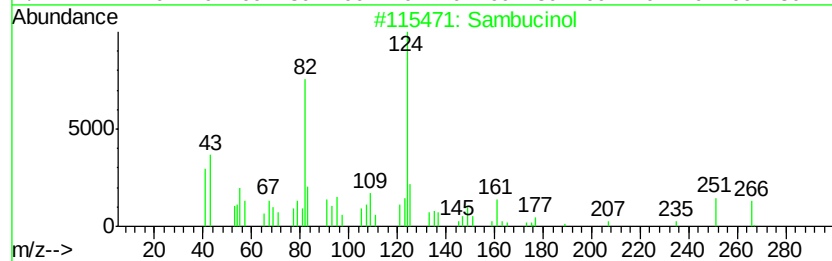
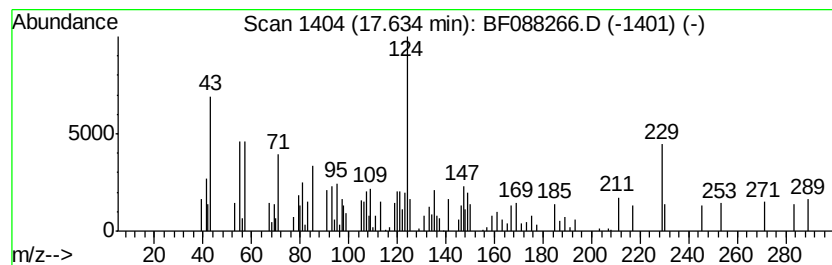
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TIC Integration Parameters: LSCINT.P

Peak Number 17 unknown17.63 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.63	4.71 ng	111586	Perylene-d12	15.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sambucinol	266	C15H22O4	090044-33-0	27
2			Thiophene-2-sulfonic acid, (3-fl...	271	C11H10FN02S2	1000311-21-1	22
3			2-Chloro-4-fluorobenzvlamide	159	C7H7ClFN	1000343-00-9	18
4			Phenol, 2,6-diamino-	124	C6H8N2O	022440-82-0	16
5			3,6-Dimethyl-5-hepten-1-ol acetate	184	C11H20O2	1000131-31-1	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062216\
Data File : BF088266.D
Acq On : 22 Jun 2016 23:12
Operator : UM/SJ
Sample : H3660-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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...	4.72	17.9	ng	404354	1	6.60	450946	20.0
3-Chloro-6-fluoro...	6.38	73.5	ng	1656120	1	6.60	450946	20.0
n-Hexadecanoic acid	11.67	2.3	ng	64859	4	11.12	574781	20.0
Trifluoroacetoxy ...	13.61	5.4	ng	150637	5	13.75	558290	20.0
n-Tetracosanol-1	14.25	5.0	ng	140031	5	13.75	558290	20.0
Oxirane, heptadecyl-	14.64	6.7	ng	159542	6	15.11	474326	20.0
Nonadecane	14.81	3.7	ng	87402	6	15.11	474326	20.0
n-Nonadecanol-1	14.85	7.5	ng	177213	6	15.11	474326	20.0
Octadecanal	15.30	4.1	ng	96539	6	15.11	474326	20.0
Hexacosane	15.50	7.0	ng	165923	6	15.11	474326	20.0
Oxirane, hexadecyl-	16.15	5.4	ng	128826	6	15.11	474326	20.0
unknown17.63	17.63	4.7	ng	111586	6	15.11	474326	20.0