LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

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-BF012417.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	5.150	266	268	271	rBV	568566	639007	12.77%	1.519%
2	5.242	274	276	279	rVB	264076	252971	5.05%	0.601%
3	5.562	301	304	307	rBV	2451213	2260641	45.17%	5.373%
4	6.590	391	394	396	rBV	1470327	1612382	32.21%	3.832%
5	6.727	404	406	409	rBV	2824555	4001454	79.95%	9.510%
6	6.819	409	414	418	rVB2	48130	99289	1.98%	0.236%
7	6.967	424	427	429	rBV	1207704	1055421	21.09%	2.508%
8	7.127	438	441	443	rBV	3704694	3599805	71.92%	8.555%
9	7.539	473	477	479	rVB	2632640	3411439	68.16%	8.107%
10	8.133	525	529	531	rBV2	19346	52316	1.05%	0.124%
11	8.259	538	540	543	rVB	1499159	1333707	26.65%	3.170%
12	8.476	557	559	560	rBV	160862	190988	3.82%	0.454%
13	8.510	560	562	563	rVB	156647	211659	4.23%	0.503%
14	8.830	588	590	591	rBV	50356	58133	1.16%	0.138%
15	8.853	591	592	594	rVB	63969	51778	1.03%	0.123%
16	9.345	632	635	637	rBV	4680532	5005222	100.00%	11.895%
17	9.379	637	638	640	rVV	71291	84455	1.69%	0.201%
18	9.448	642	644	646	rVB2	33643	51086	1.02%	0.121%
19	9.539	651	652	655	rVB	61098	58850	1.18%	0.140%
20	9.733	667	669	672	rVB	581213	601962	12.03%	1.431%
21	10.019	692	694	697	rBV	1188875	1490841	29.79%	3.543%
22	10.168	704	707	710	rBV	52539	91460	1.83%	0.217%
23	10.248	713	714	716	rVV	88209	69282	1.38%	0.165%
24	10.316	718	720	723	rVV	58796	64853	1.30%	0.154%
25	10.453	729	732	734	rBV2	76146	129411	2.59%	0.308%
26	10.533	736	739	741	rBV2	63103	89884	1.80%	0.214%
27	10.682	749	752	755	rBV4	68837	142051	2.84%	0.338%
28	10.751	755	758	760	rBV4	45743	89009	1.78%	0.212%
29	10.819	760	764	766	rBV	2744648	3172214	63.38%	7.539%
30	10.945	772	775	778	rVB2	134512	215561	4.31%	0.512%
31	11.002	778	780	781	rBV	94301	146399	2.92%	0.348%
32	11.025	781	782	784	rVV2	169293	210991	4.22%	0.501%
33	11.059	784	785	787	rVV2	146767	184936	3.69%	0.440%
34	11.128	789	791	794	rVV2	99792	230460	4.60%	0.548%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

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-BF012417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.174	794	795	797	rVV2	224674	238294	4.76%	0.566%
36	11.219	797	799	801	rVV2	115573	210533	4.21%	0.500%
37	11.254	801	802	804	rVB	123845	101592	2.03%	0.241%
38	11.379	811	813	814	rBV	135956	134086	2.68%	0.319%
39	11.516	822	825	827	rBV	1734062	1611545	32.20%	3.830%
40	11.722	841	843	845	rVB	104853	104777	2.09%	0.249%
41	11.768	845	847	849	rBV2	54806	100499	2.01%	0.239%
42	11.985	864	866	869	rVB	52020	80557	1.61%	0.191%
43	12.042	869	871	875	rBV2	375493	406151	8.11%	0.965%
44	12.831	938	940	943	rBV	187279	215147	4.30%	0.511%
45	12.877	943	944	947	rVV	107282	108715	2.17%	0.258%
46	12.922	947	948	952	rVB2	48064	58183	1.16%	0.138%
47	12.979	952	953	956	rBV	42251	60452	1.21%	0.144%
48	13.105	961	964	967	rBV	4062769	4462212	89.15%	10.605%
49	13.665	1011	1013	1015	rBV	70289	64469	1.29%	0.153%
50	13.882	1030	1032	1040	rVB	41481	71962	1.44%	0.171%
51	13.997	1040	1042	1048	rBV	218069	252967	5.05%	0.601%
52	14.157	1053	1056	1058	rBV	1464375	1460572	29.18%	3.471%
53	15.631	1182	1185	1188	rBV	716278	1060360	21.19%	2.520%
54	16.123	1225	1228	1231	rVB	46002	80850	1.62%	0.192%
55	16.637	1270	1273	1277	rBV	47626	100054	2.00%	0.238%
56	17.243	1323	1326	1330	rVB3	31106	69706	1.39%	0.166%
57	17.963	1387	1389	1394	rVB2	26824	63992	1.28%	0.152%

Sum of corrected areas: 42077592

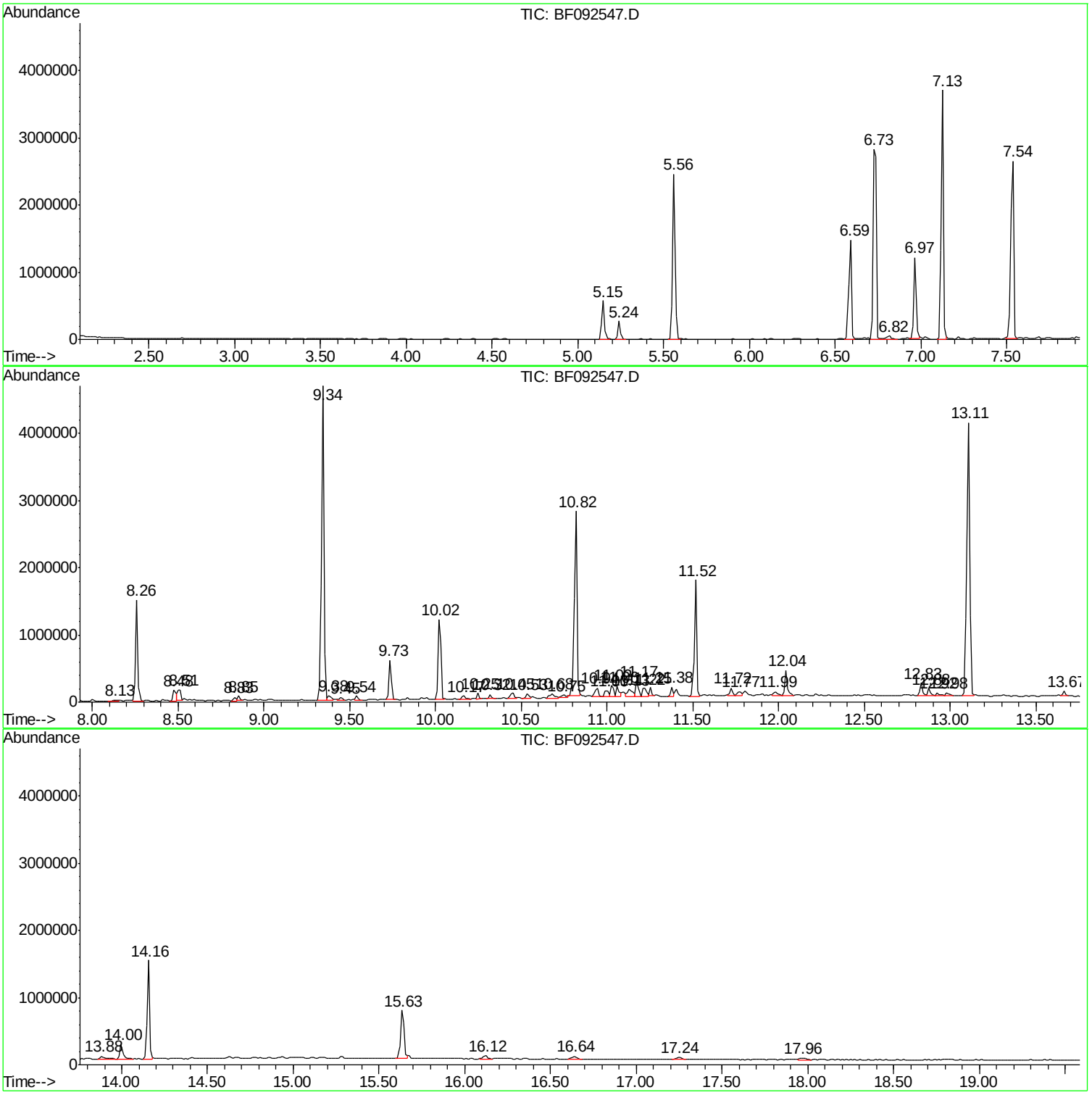
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

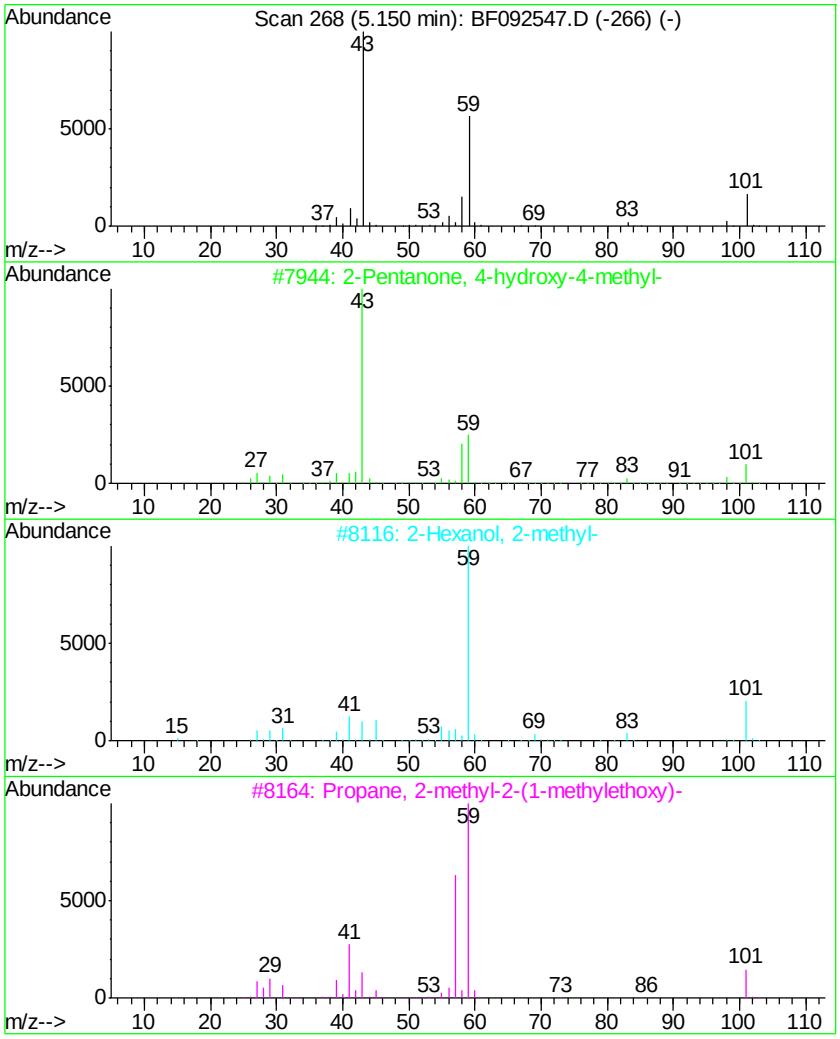
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

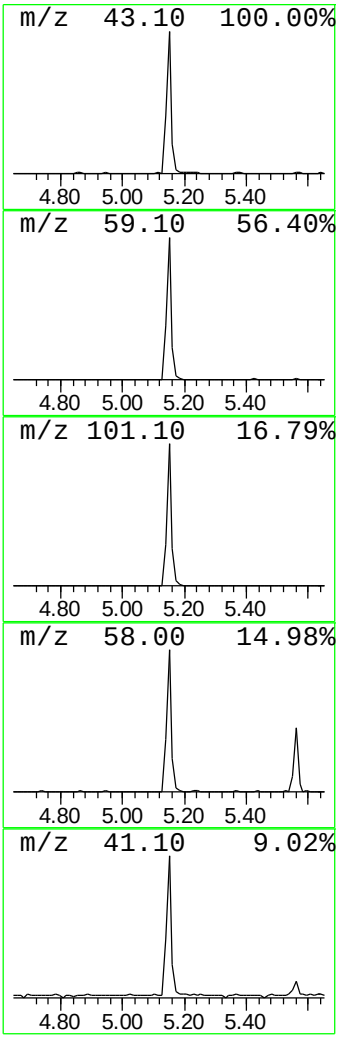
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	12.11 ng	639007	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

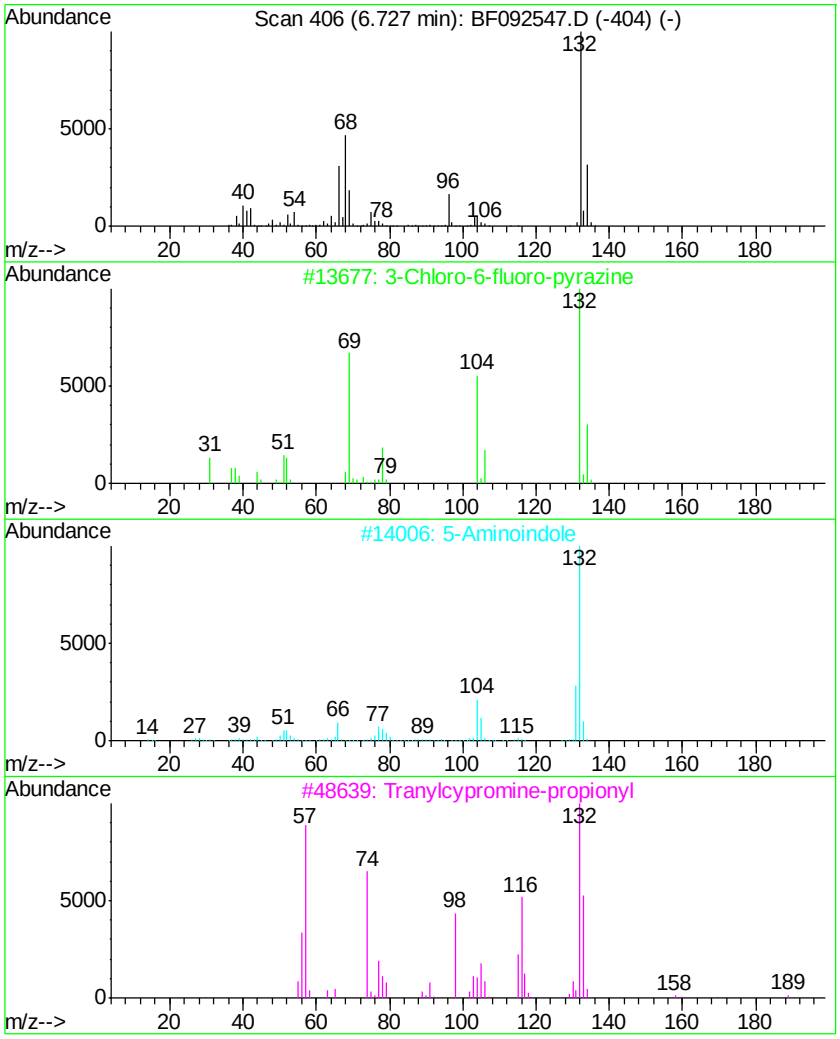
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

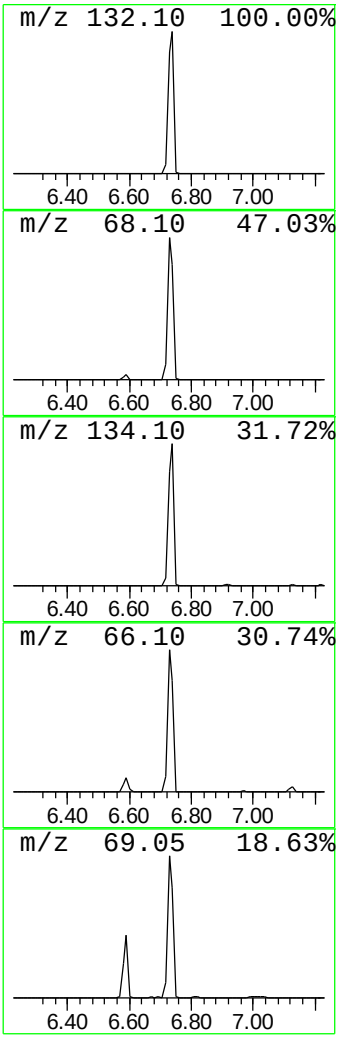
****

Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	75.83 ng	4001450	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

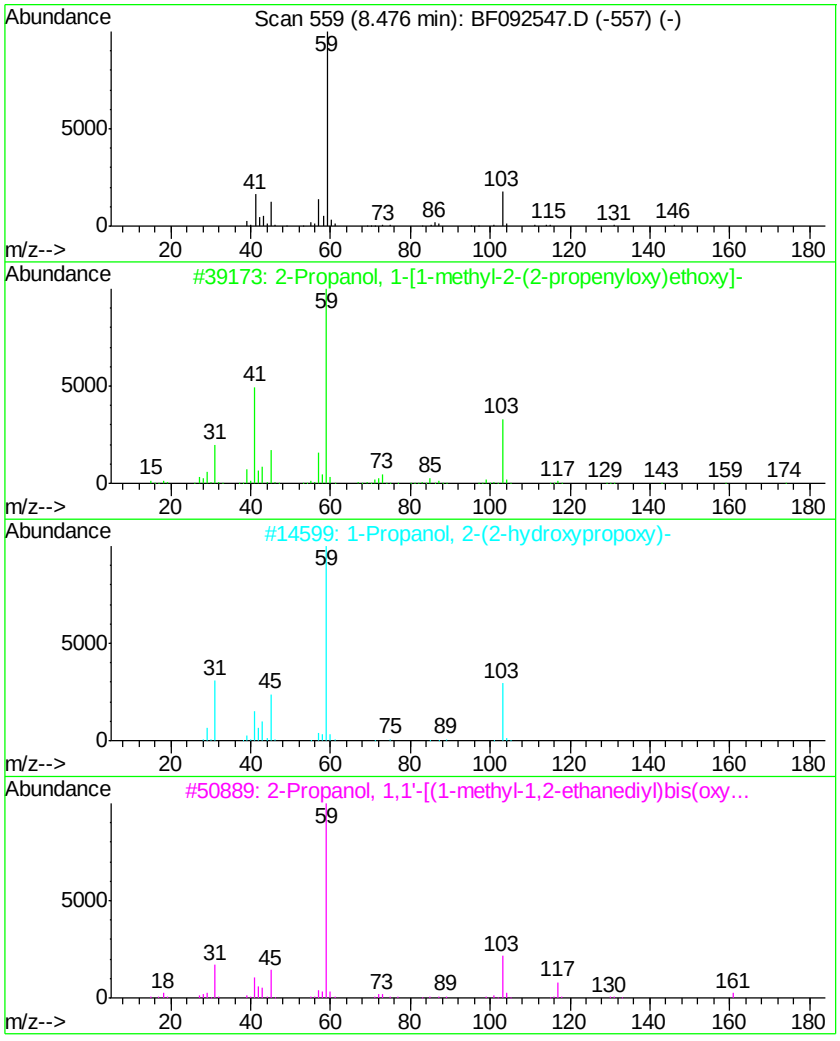
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

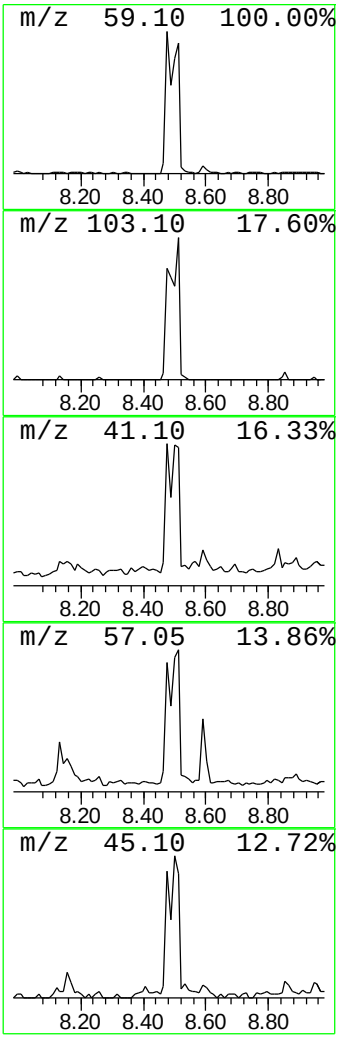
****

Peak Number 5 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.48	2.86 ng	190988	Naphthalene-d8	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	56
4	Propanedioic acid, oxo-, dimethy...	146	C5H6O5	003298-40-6	53
5	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

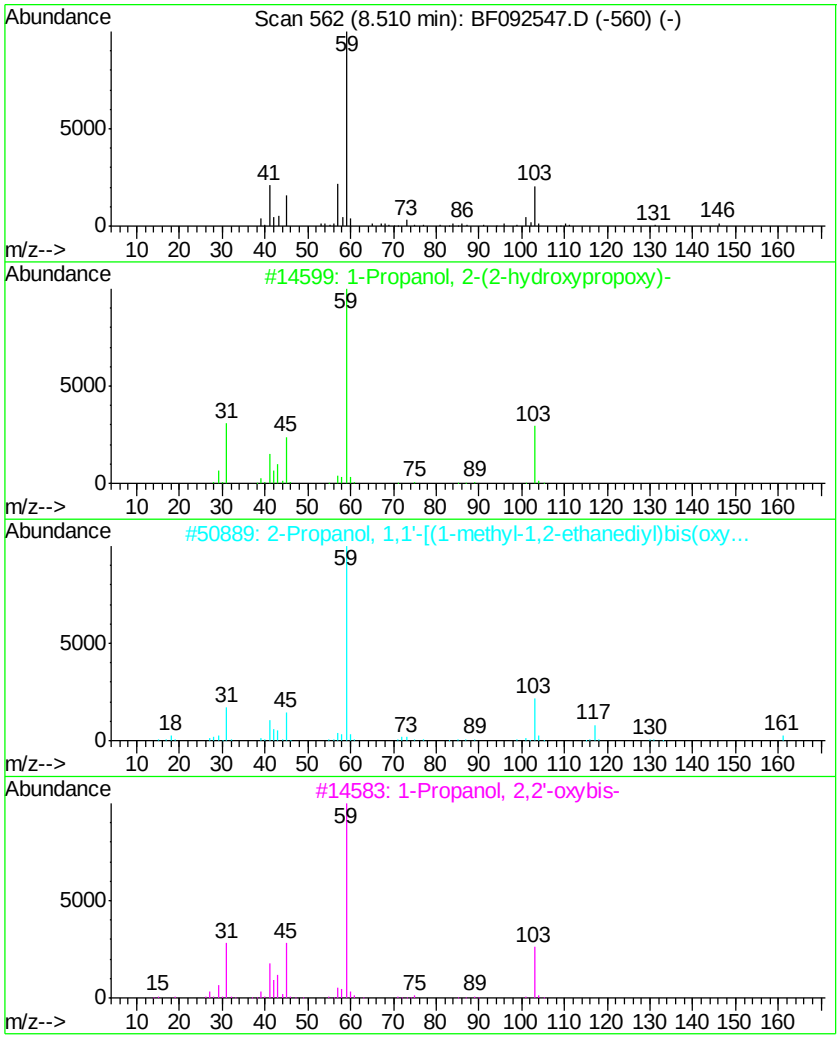
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

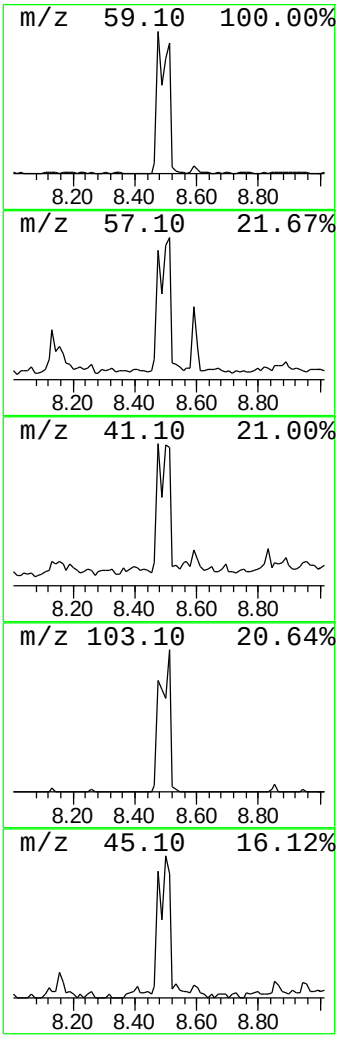
****

Peak Number 6 1-Propanol, 2-(2-hydroxypro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.51	3.17 ng	211659	Naphthalene-d8	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
2	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	72
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72
4	Propane, 1,2-dimethoxy-	104	C5H12O2	007778-85-0	58
5	Dipropylene glycol	134	C6H14O3	025265-71-8	56





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

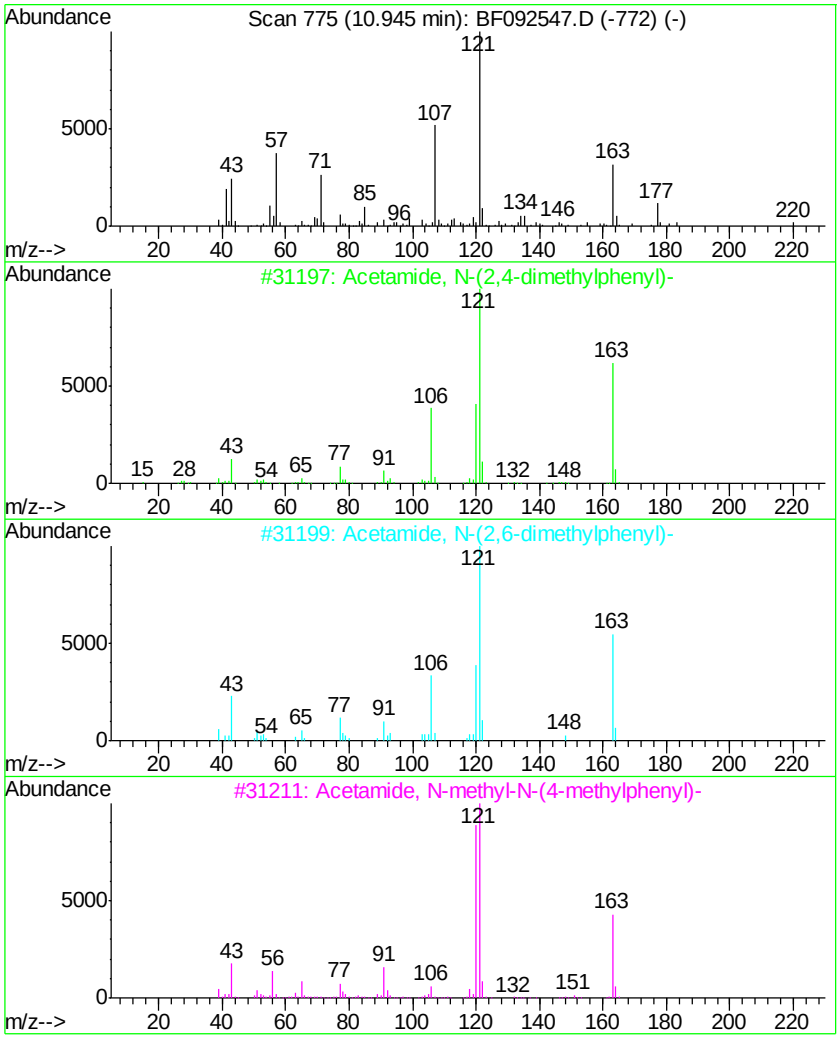
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

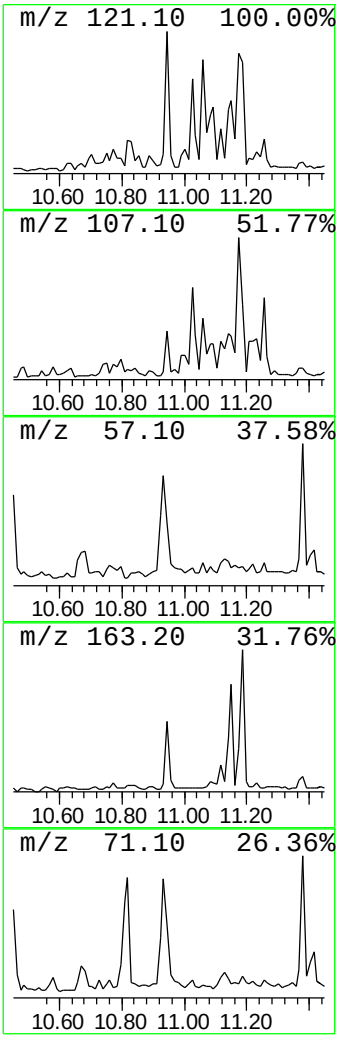
****

Peak Number 7 unknown10.95 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	2.68 ng	215561	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(2,4-dimethylphenyl)-	163	C10H13NO	002050-43-3	46
2	Acetamide, N-(2,6-dimethylphenyl)-	163	C10H13NO	002198-53-0	43
3	Acetamide, N-methyl-N-(4-methylp...	163	C10H13NO	000612-03-3	43
4	2-Acetamidotropone	163	C9H9NO2	006422-12-4	43
5	2-Propanone, 1-(4-methoxyphenyl)-	164	C10H12O2	000122-84-9	38





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Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

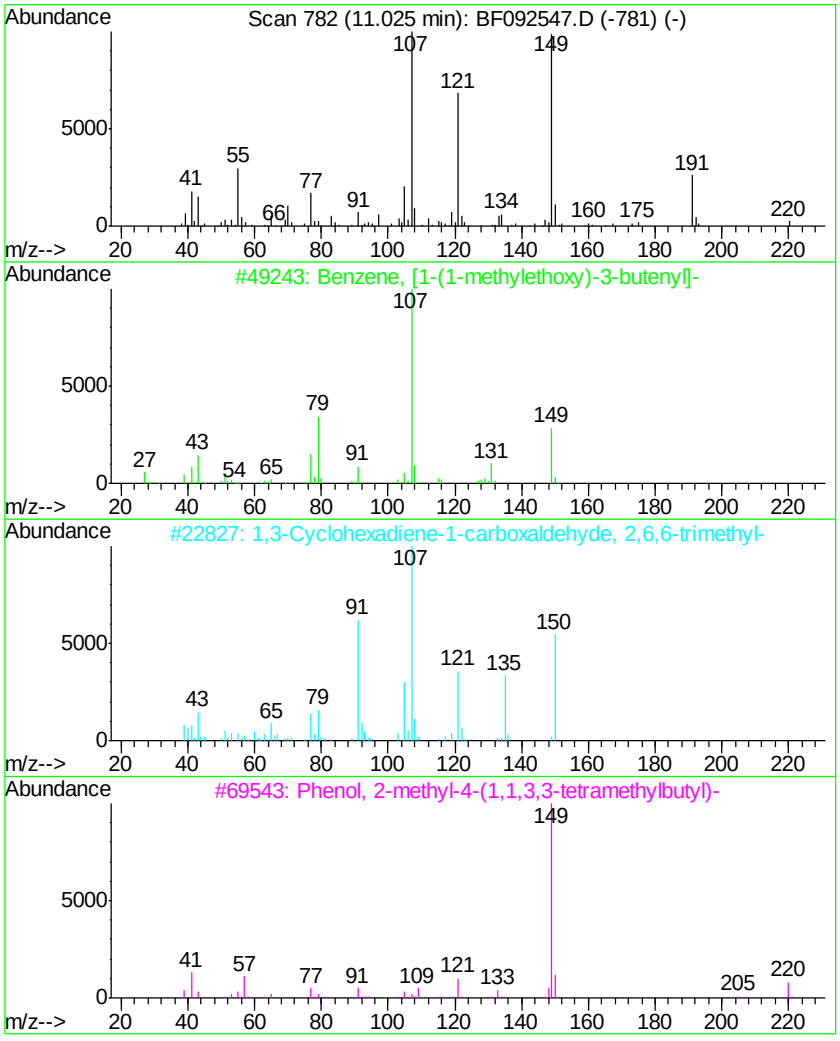
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

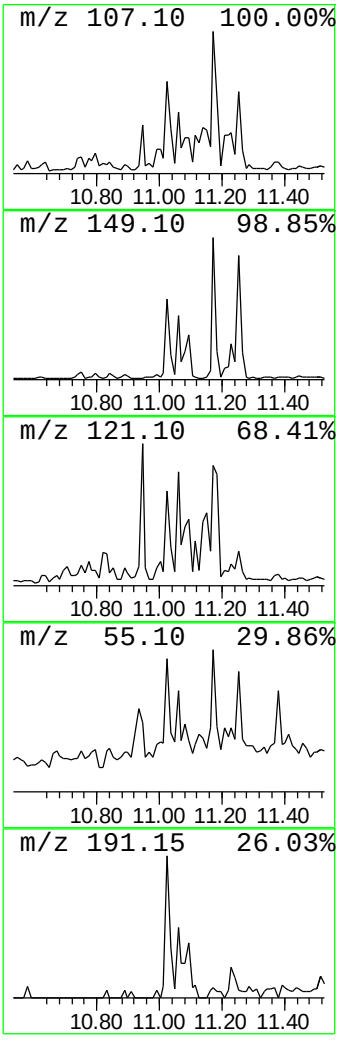
****

Peak Number 8 Benzene, [1-(1-methylethoxy... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.03	2.62 ng	210991	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, [1-(1-methylethoxy)-3-b...	190	C13H18O	098088-47-2	59
2	1,3-Cyclohexadiene-1-carboxaldeh...	150	C10H14O	000116-26-7	38
3	Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	35
4	1,3-Dioxolane, 2-tert-butyl-2-ph...	206	C13H18O2	006135-60-0	35
5	Phenol, 4-(1,1-dimethylethyl)-2-...	164	C11H16O	000098-27-1	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

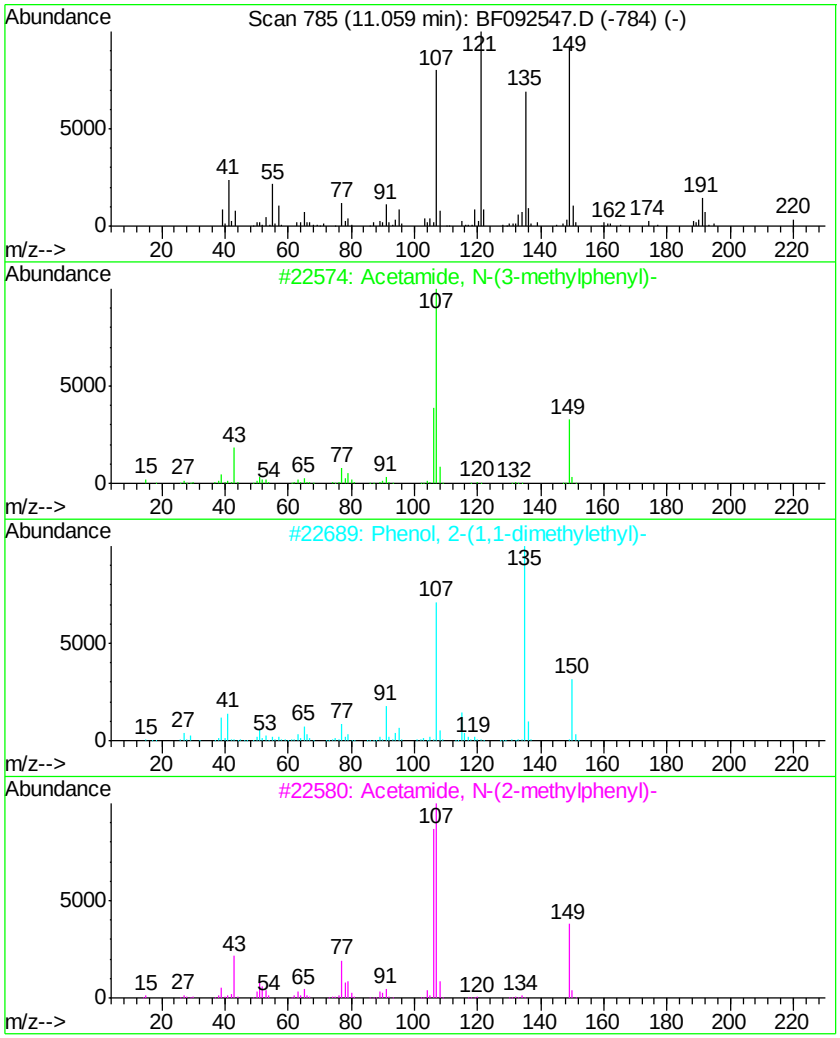
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

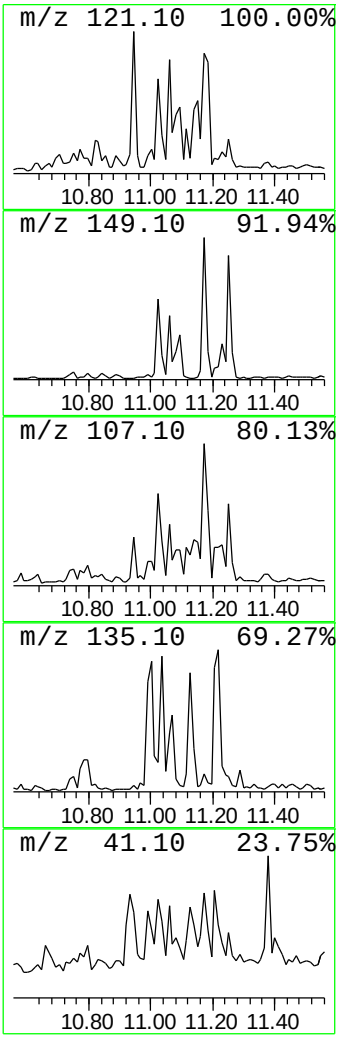
****

Peak Number 9 unknown11.06 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.06	2.30 ng	184936	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	43
2	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	38
3	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	25
4	Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	25
5	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

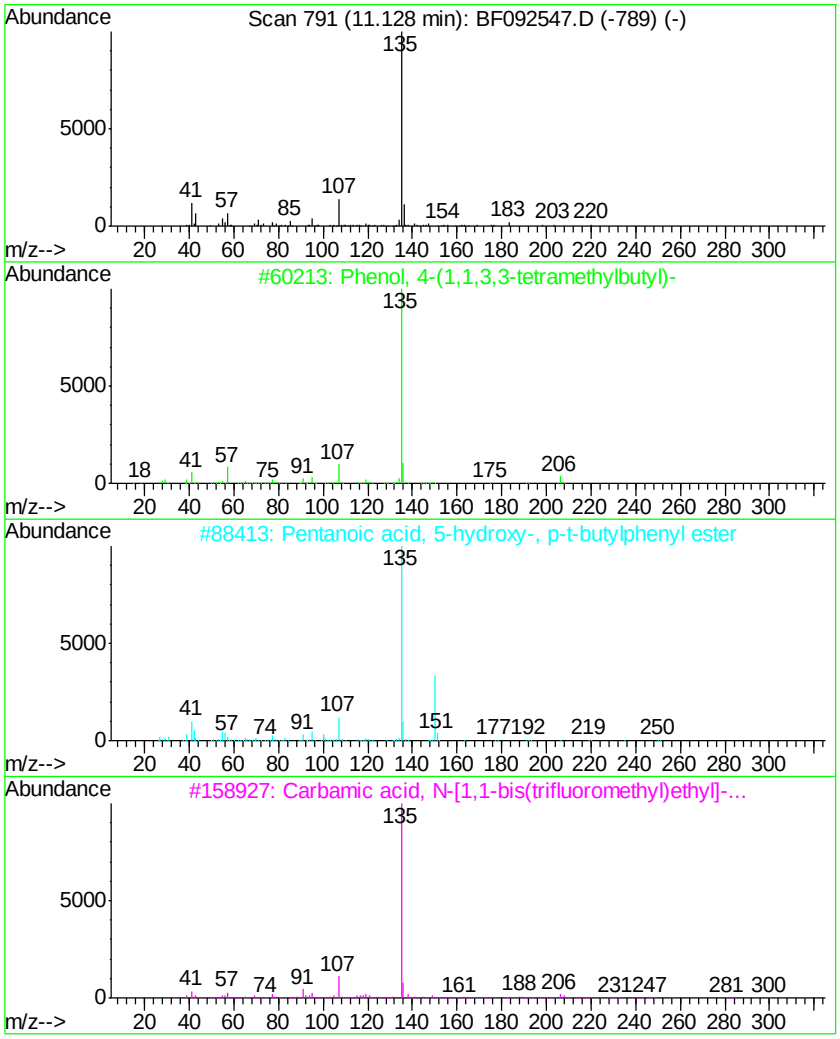
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

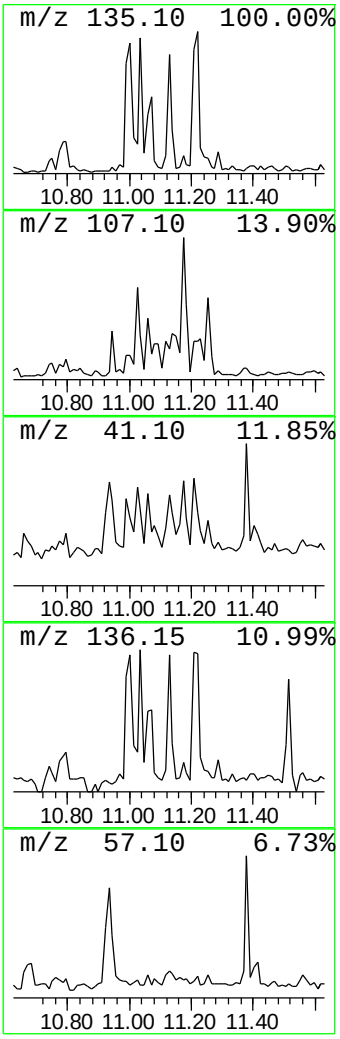
****

Peak Number 10 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.13	2.86 ng	230460	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
2	Pentanoic acid, 5-hydroxy-, p-t-...	250	C15H22O3	166273-37-6	56
3	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	56
4	2-Methyl-2-(4'-hydroxyphenyl)pen...	192	C12H16O2	070205-18-4	56
5	1-Pentanone, 1-(4-methoxyphenyl)...	207	C12H17NO2	055937-94-5	50





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Data File : BF092547.D
Acq On : 27 Jan 2017 1:32
Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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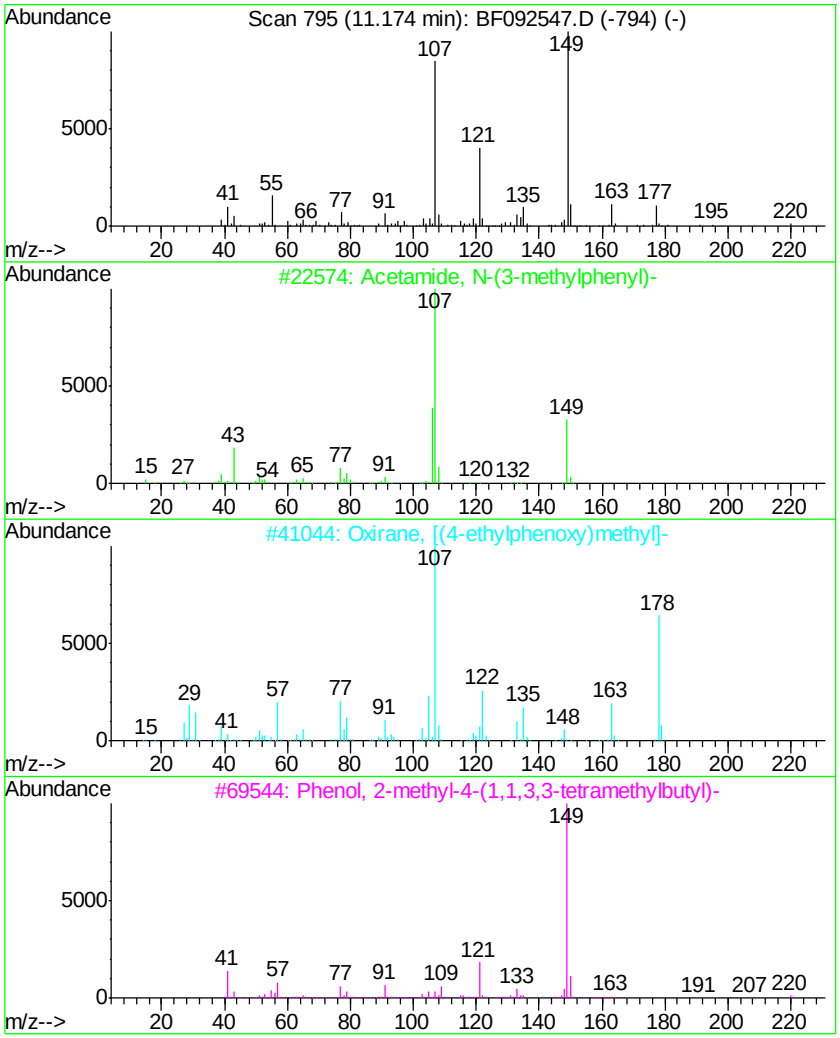
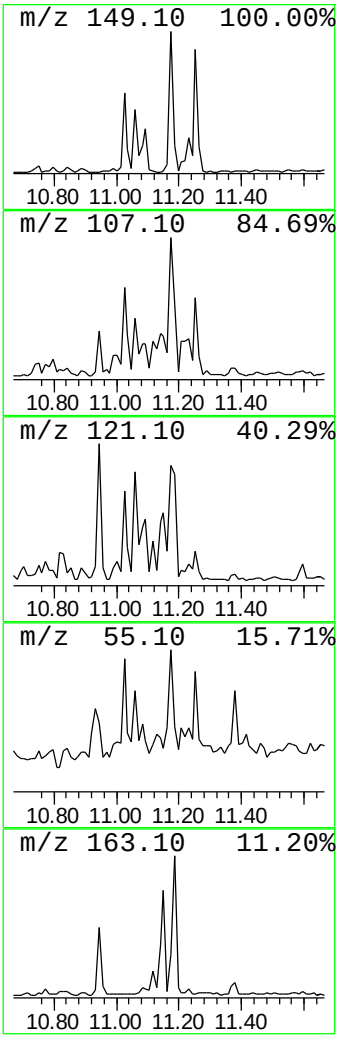
Peak Number 11 Acetamide, N-(3-methylphenyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	2.96 ng	238294	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	64
2	Oxirane, [(4-ethylphenoxy)methyl]-	178	C11H14O2	002930-02-1	45
3	Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	43
4	1,3-Cyclopentadiene, 5,5-dimethy...	178	C13H22	1000163-88-0	37
5	Phenol, 4-(1,1-dimethylethyl)-2-...	164	C11H16O	000098-27-1	32





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Misc :
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Instrument : BNA_F
ClientSampleId : W-33

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TIC Integration Parameters: LSCINT.P

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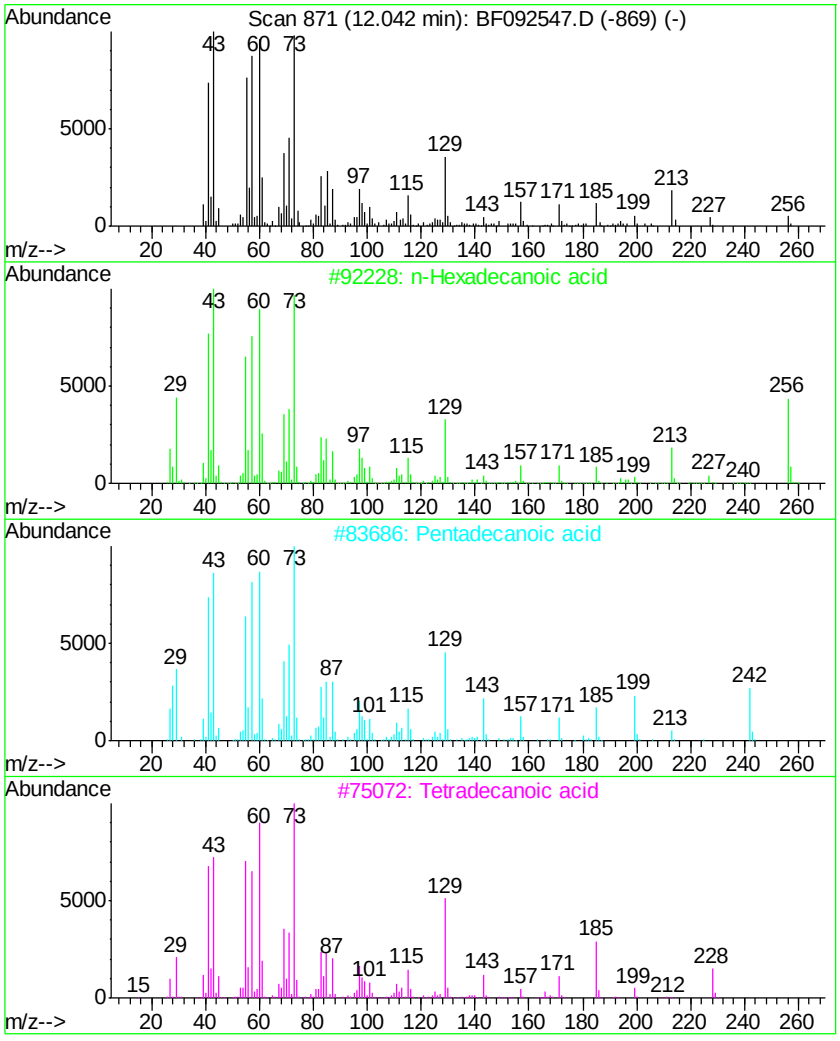
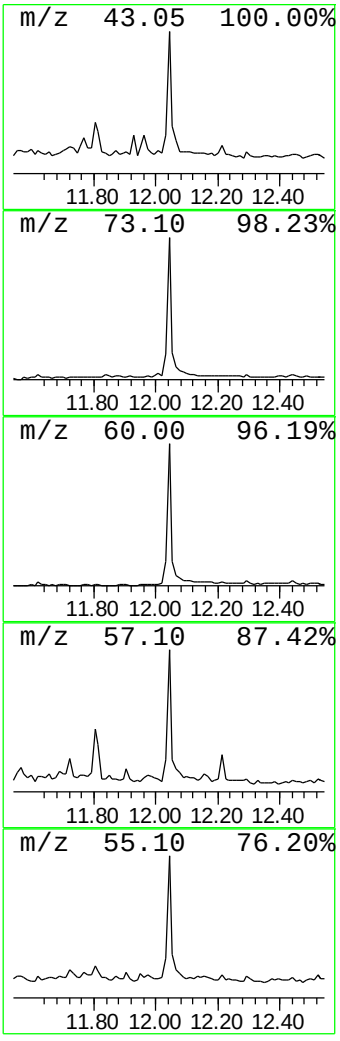
Peak Number 13 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	5.04 ng	406151	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Dodecane	170	C12H26	000112-40-3	11





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Operator : SJ/MA
Sample : I1451-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
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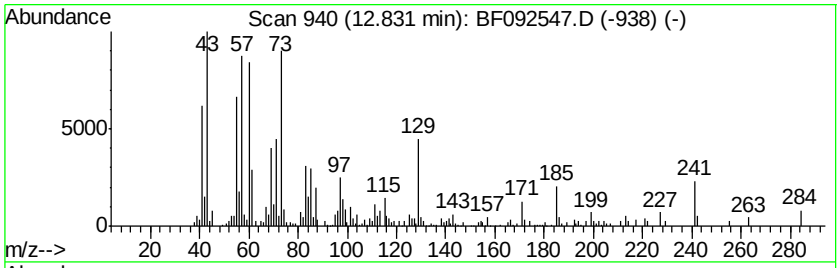
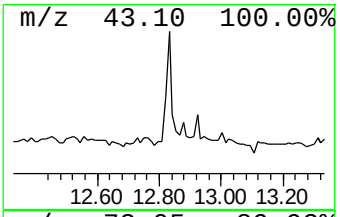
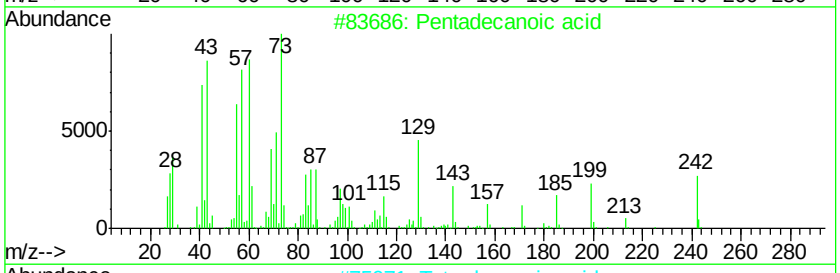
Peak Number 14 Pentadecanoic acid Concentration Rank 12

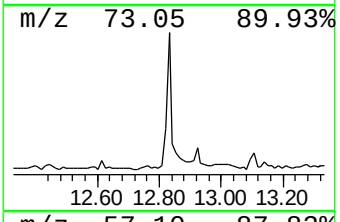
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	2.67 ng	215147	Phenanthrene-d10	11.52

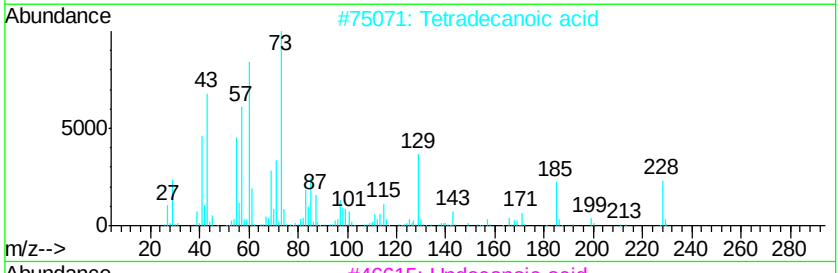
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Undecanoic acid	186	C11H22O2	000112-37-8	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38

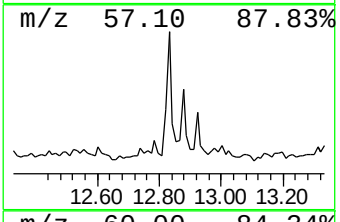


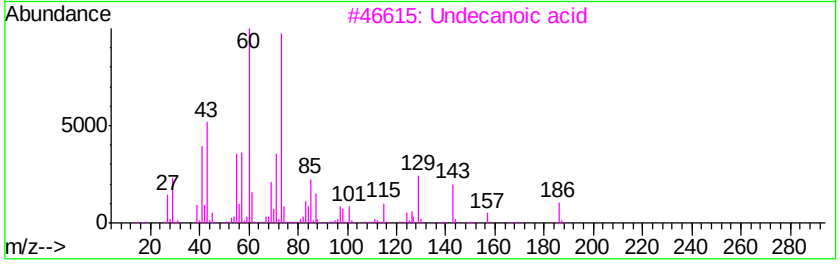


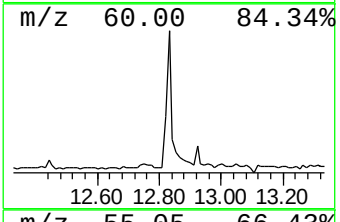


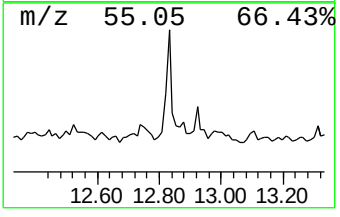












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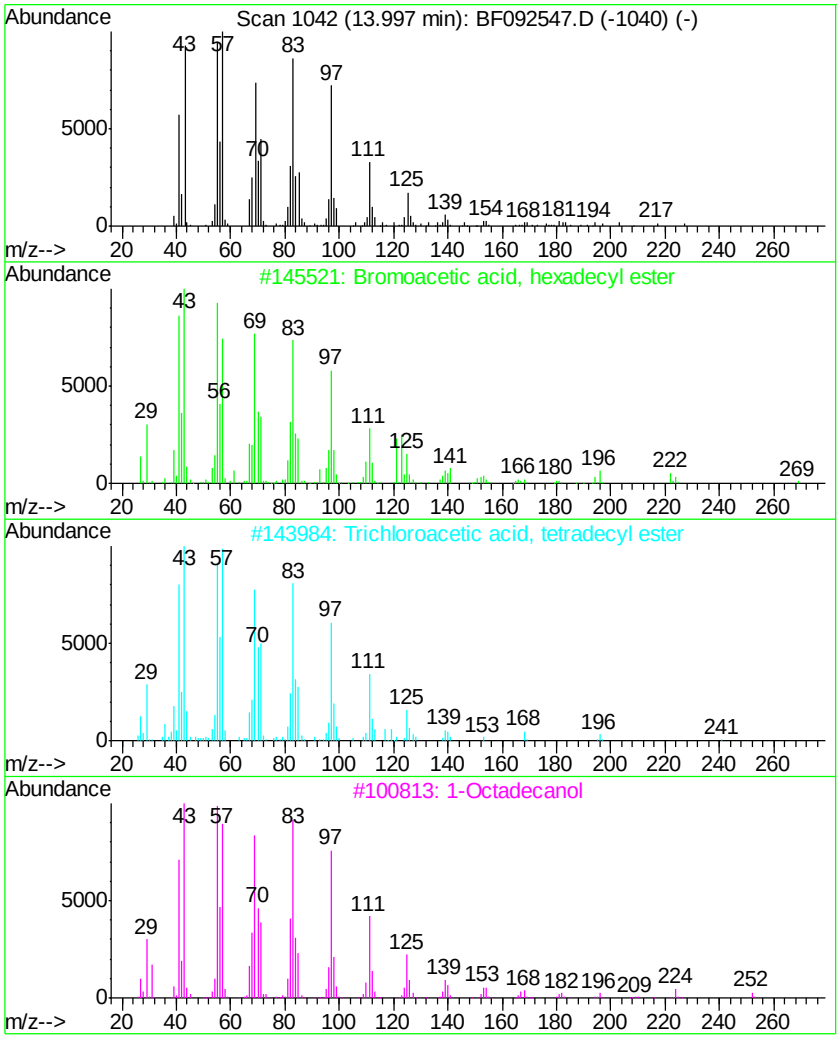
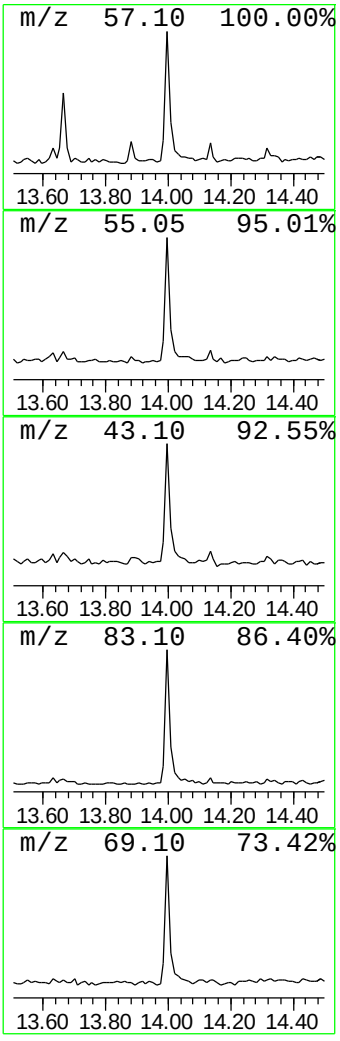
****

Peak Number 15 Bromoacetic acid, hexadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	3.46 ng	252967	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3	1-Octadecanol	270	C18H38O	000112-92-5	90
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	87
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	12.1	ng	639007	1	6.97	1055420	20.0
unknown6.73	6.73	75.8	ng	4001450	1	6.97	1055420	20.0
2-Propanol, 1-[1-...	8.48	2.9	ng	190988	2	8.26	1333710	20.0
1-Propanol, 2-(2-...	8.51	3.2	ng	211659	2	8.26	1333710	20.0
unknown10.95	10.95	2.7	ng	215561	4	11.52	1611550	20.0
Benzene, [1-(1-me...	11.03	2.6	ng	210991	4	11.52	1611550	20.0
unknown11.06	11.06	2.3	ng	184936	4	11.52	1611550	20.0
Phenol, 4-(1,1,3,...	11.13	2.9	ng	230460	4	11.52	1611550	20.0
Acetamide, N-(3-m...	11.17	3.0	ng	238294	4	11.52	1611550	20.0
n-Hexadecanoic acid	12.04	5.0	ng	406151	4	11.52	1611550	20.0
Pentadecanoic acid	12.83	2.7	ng	215147	4	11.52	1611550	20.0
Bromoacetic acid,...	14.00	3.5	ng	252967	5	14.16	1460570	20.0