LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

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-BF063016.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	1.678	6	8	16	rVB	39866	96480	6.00%	0.644%
2	1.793	16	18	25	rVV	423700	564753	35.14%	3.771%
3	1.884	25	26	41	rVB2	36534	76982	4.79%	0.514%
4	2.867	109	112	125	rVB	20547	50099	3.12%	0.334%
5	4.856	283	286	290	rBV	141840	194805	12.12%	1.301%
6	5.301	323	325	328	rVB	1366838	1313919	81.75%	8.772%
7	6.353	415	417	420	rVB	1197199	1319661	82.11%	8.811%
8	6.479	425	428	430	rVV	1446141	1597070	99.37%	10.663%
9	6.547	430	434	440	rVB2	9922	17092	1.06%	0.114%
10	6.707	446	448	449	rBV	347735	350986	21.84%	2.343%
11	6.856	459	461	463	rVB	918235	1126354	70.08%	7.520%
12	7.267	494	497	500	rVB	801176	852044	53.01%	5.689%
13	7.519	513	519	523	rVB	4218	16228	1.01%	0.108%
14	7.987	558	560	563	rBV	507410	464844	28.92%	3.104%
15	8.433	597	599	600	rBV	18322	24334	1.51%	0.162%
16	8.593	612	613	617	rVB	16499	17341	1.08%	0.116%
17	8.708	620	623	624	rBV2	20703	28025	1.74%	0.187%
18	8.799	629	631	633	rVV	42545	33020	2.05%	0.220%
19	9.073	652	655	657	rBV	1531976	1607257	100.00%	10.731%
20	9.165	661	663	665	rVV	19094	21487	1.34%	0.143%
21	9.405	680	684	685	rBV	29427	38975	2.42%	0.260%
22	9.428	685	686	687	rVV	29540	21394	1.33%	0.143%
23	9.462	687	689	692	rVV	243092	228423	14.21%	1.525%
24	9.553	695	697	699	rVB	12857	20898	1.30%	0.140%
25	9.690	707	709	711	rVB	23461	21572	1.34%	0.144%
26	9.736	711	713	716	rBV	428197	414683	25.80%	2.769%
27	9.942	730	731	733	rVB	22865	18988	1.18%	0.127%
28	10.148	747	749	751	rBV2	26042	28450	1.77%	0.190%
29	10.182	751	752	754	rVB	30016	24869	1.55%	0.166%
30	10.399	769	771	773	rBV	18125	20136	1.25%	0.134%
31	10.525	780	782	784	rBV	824467	744863	46.34%	4.973%
32	10.673	792	795	797	rBV	54834	94223	5.86%	0.629%
33	10.856	808	811	814	rBV3	8521	22261	1.39%	0.149%
34	10.971	817	821	824	rBV3	74449	124801	7.76%	0.833%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.096	831	832	834	rBV	33146	45964	2.86%	0.307%
36	11.211	840	842	846	rVB	331591	351096	21.84%	2.344%
37	11.531	868	870	873	rVB	19332	23633	1.47%	0.158%
38	11.759	885	890	892	rBV2	43960	74669	4.65%	0.499%
39	11.816	892	895	899	rVV	48448	81173	5.05%	0.542%
40	11.931	903	905	909	rVV	22354	26476	1.65%	0.177%
41	12.011	910	912	917	rVB3	9984	17293	1.08%	0.115%
42	12.262	932	934	936	rBV	21818	21446	1.33%	0.143%
43	12.319	938	939	940	rVB	26813	18486	1.15%	0.123%
44	12.422	945	948	950	rBV	37692	43695	2.72%	0.292%
45	12.639	964	967	969	rBV	28590	34185	2.13%	0.228%
46	12.685	969	971	975	rVB2	12264	26089	1.62%	0.174%
47	12.799	979	981	983	rBV	1149296	1017869	63.33%	6.796%
48	12.948	990	994	998	rBV2	8029	25273	1.57%	0.169%
49	13.039	998	1002	1004	rBV2	16021	32161	2.00%	0.215%
50	13.074	1004	1005	1009	rVB2	14318	18474	1.15%	0.123%
51	13.165	1009	1013	1015	rBV2	8879	23145	1.44%	0.155%
52	13.382	1027	1032	1035	rBV2	30606	55653	3.46%	0.372%
53	13.474	1037	1040	1045	rBV	16439	33601	2.09%	0.224%
54	13.588	1047	1050	1052	rBV2	11756	20068	1.25%	0.134%
55	13.702	1057	1060	1064	rVV	105611	125047	7.78%	0.835%
56	13.839	1069	1072	1074	rBV	455832	465824	28.98%	3.110%
57	14.331	1113	1115	1121	rBV	61205	100558	6.26%	0.671%
58	14.560	1133	1135	1137	rBV3	11331	18562	1.15%	0.124%
59	14.628	1139	1141	1144	rVV	22383	46104	2.87%	0.308%
60	14.685	1144	1146	1148	rVB	22635	31071	1.93%	0.207%
61	14.834	1156	1159	1164	rVB	32233	65661	4.09%	0.438%
62	14.925	1165	1167	1170	rBV2	22309	38014	2.37%	0.254%
63	15.097	1180	1182	1185	rVB	22996	31536	1.96%	0.211%
64	15.154	1185	1187	1189	rBV	18429	24330	1.51%	0.162%
65	15.211	1189	1192	1195	rVV	280075	310696	19.33%	2.074%
66	15.257	1195	1196	1200	rVB3	12430	16766	1.04%	0.112%
67	15.645	1228	1230	1232	rBV	14092	18801	1.17%	0.126%
68	16.651	1316	1318	1323	rVB5	21868	40262	2.51%	0.269%
69	18.811	1504	1507	1513	rVB6	19710	56811	3.53%	0.379%

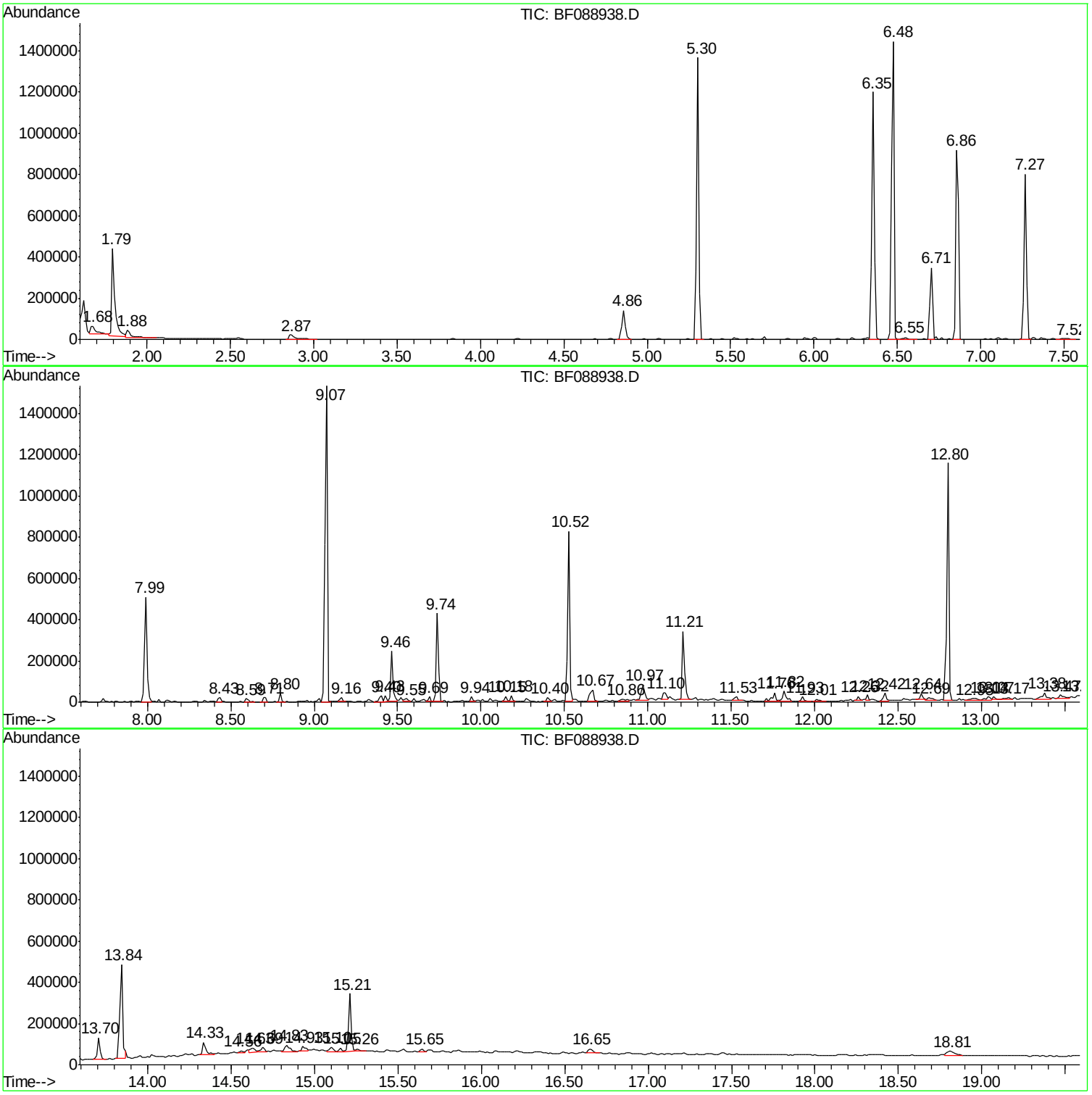
Sum of corrected areas: 14977809

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

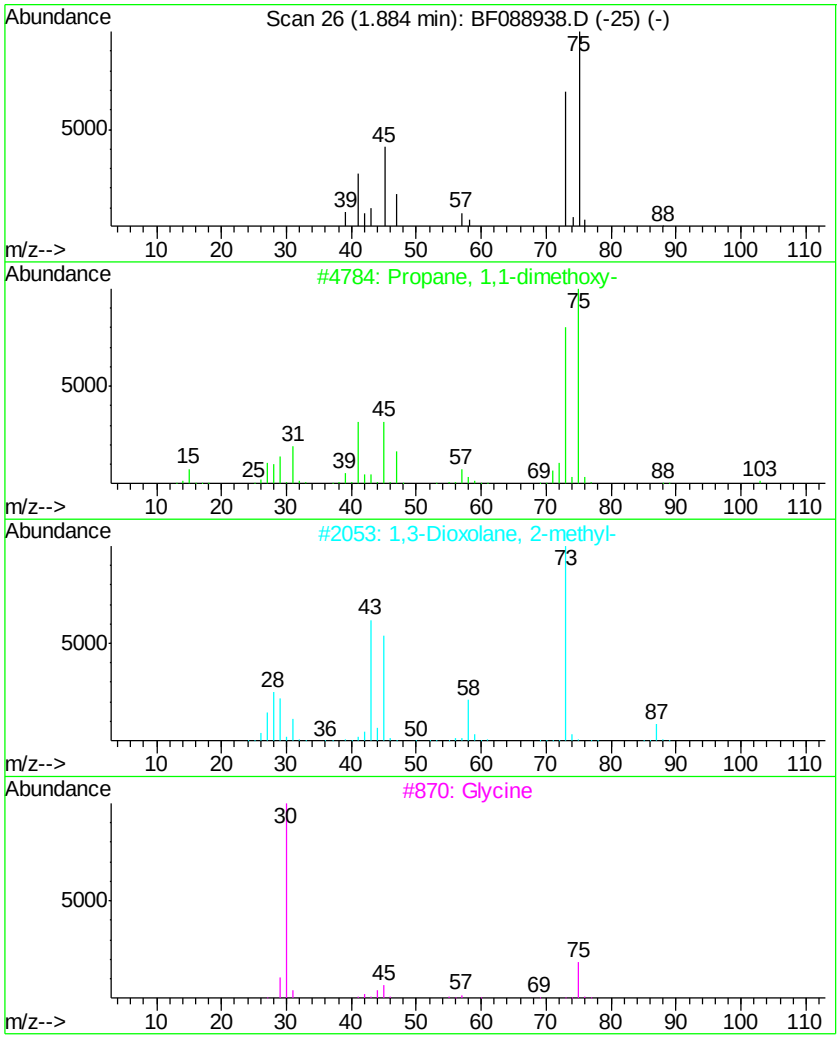
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

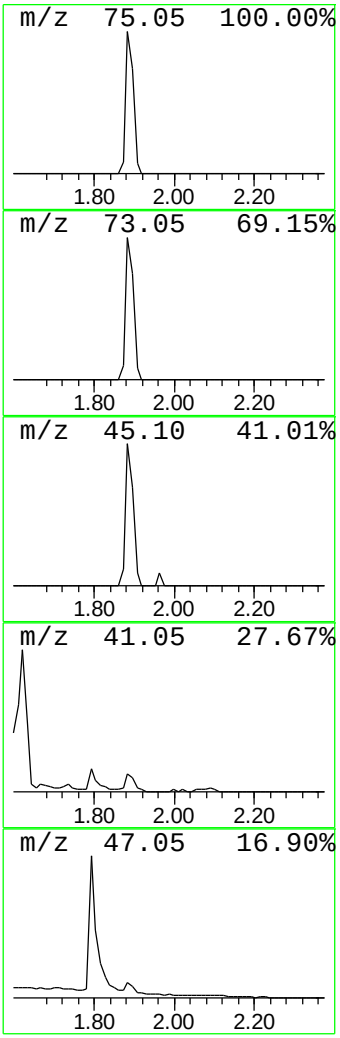
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.88	4.39 ng	76982	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
3	Glycine	75	C2H5NO2	000056-40-6	7
4	1-Propene-1-thiol	74	C3H6S	000925-89-3	5
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

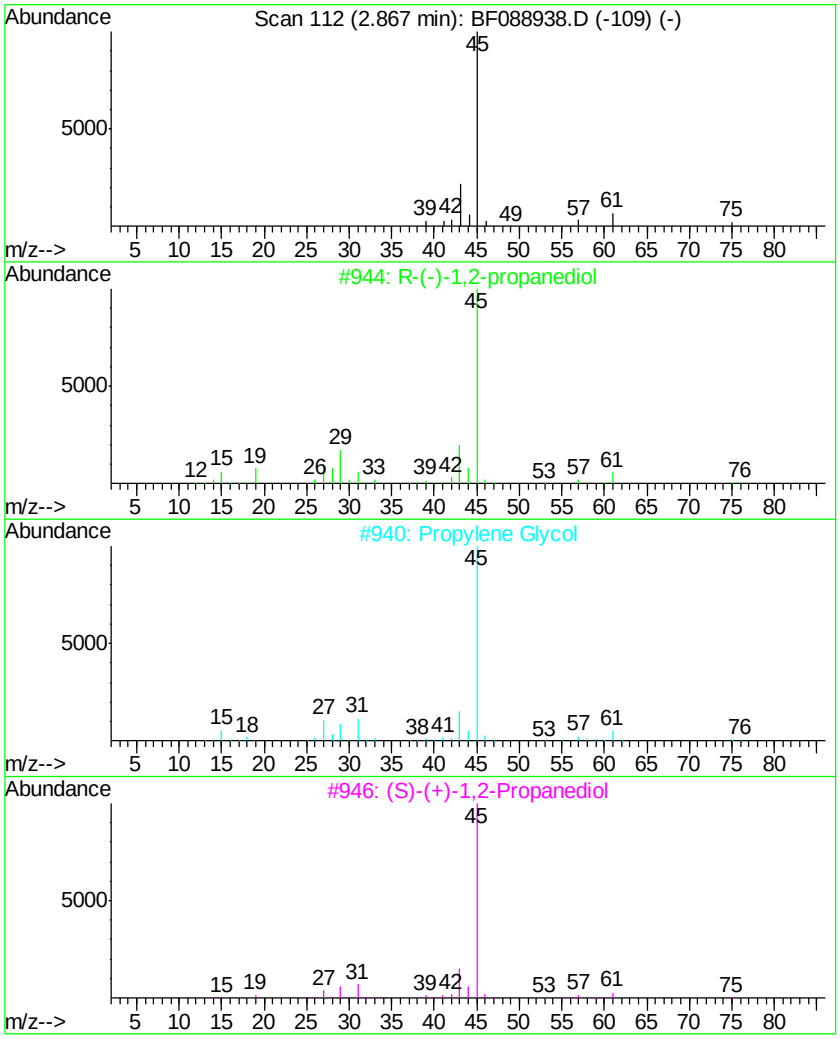
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

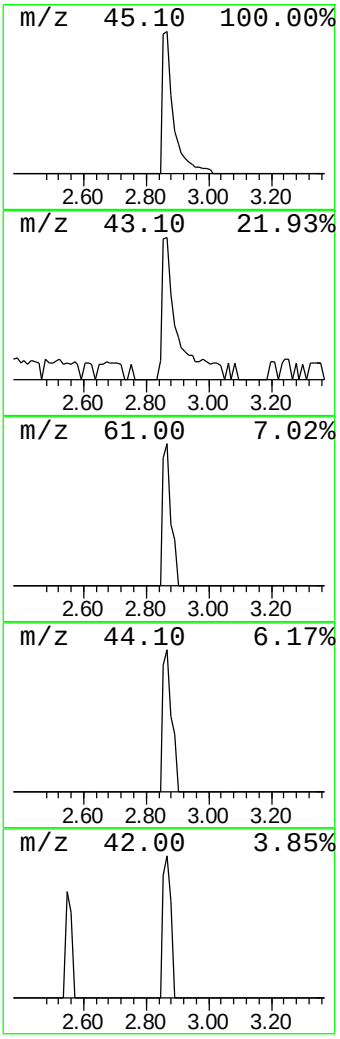
****

Peak Number 4 R-(-)-1,2-propanediol Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	2.85 ng	50099	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

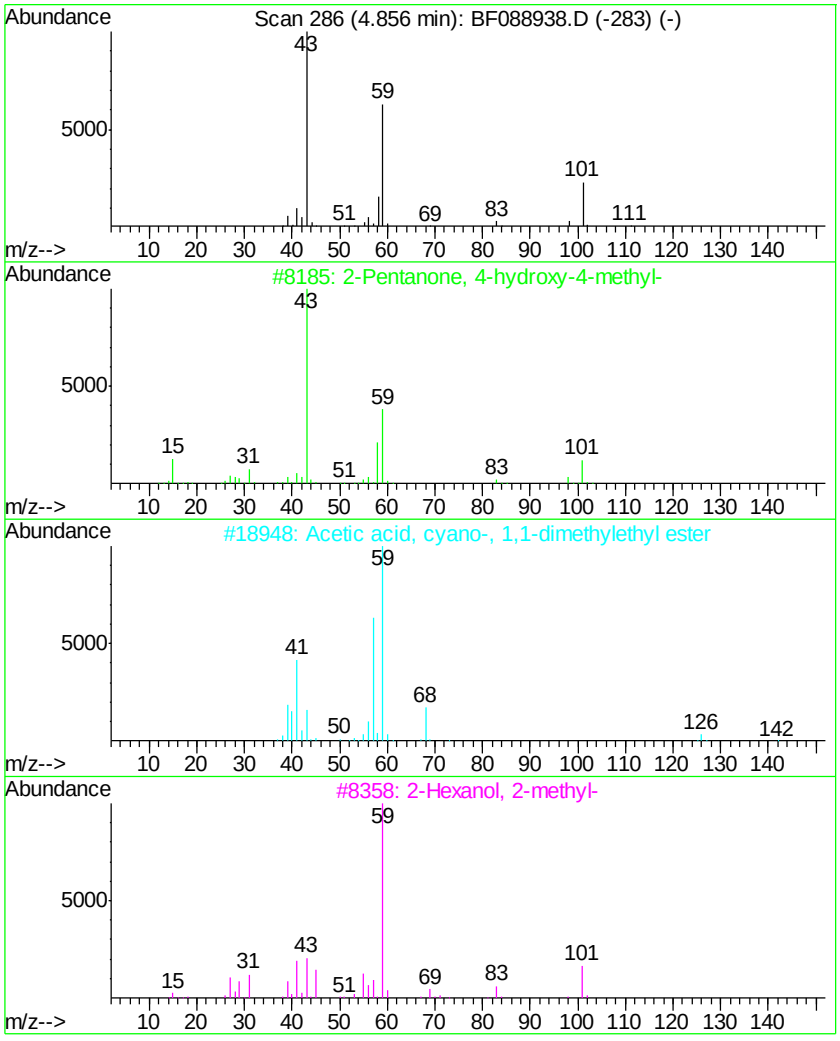
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

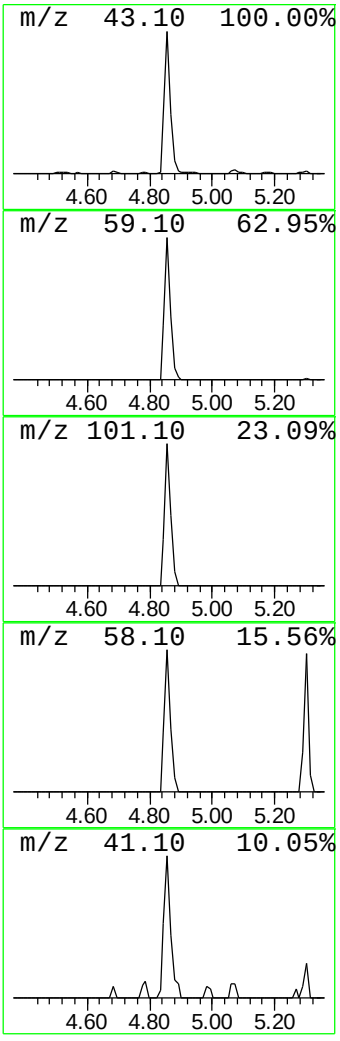
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	11.10 ng	194805	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

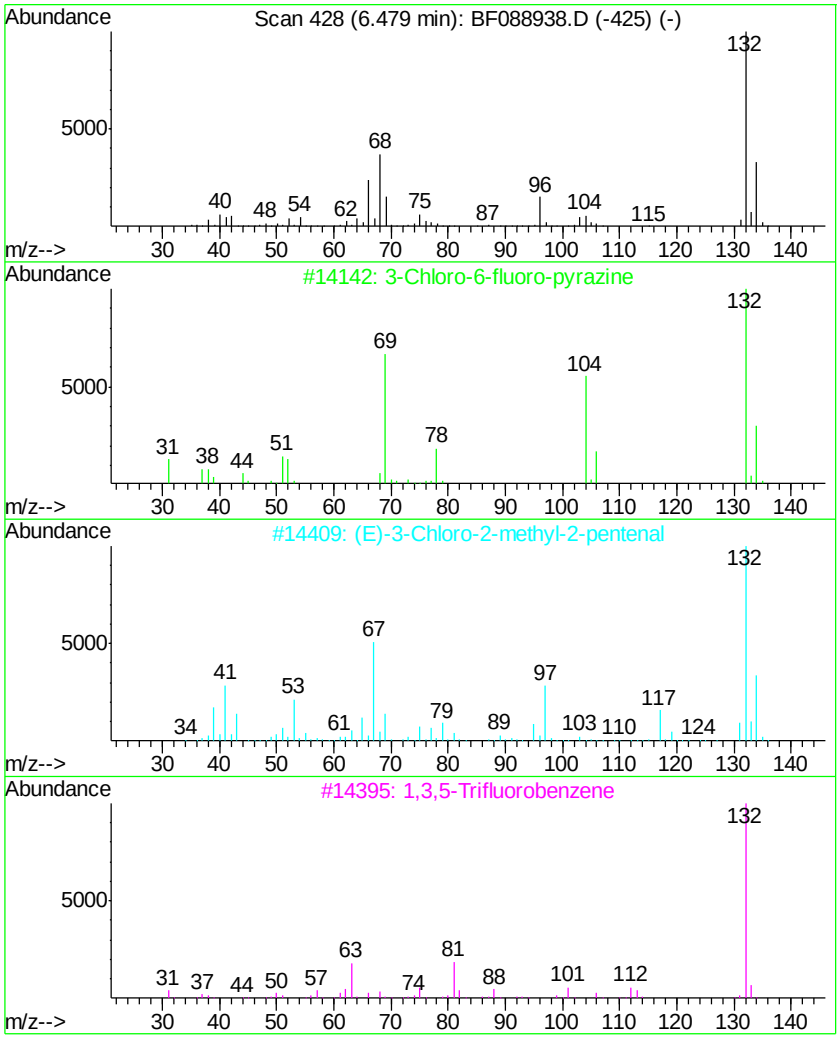
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

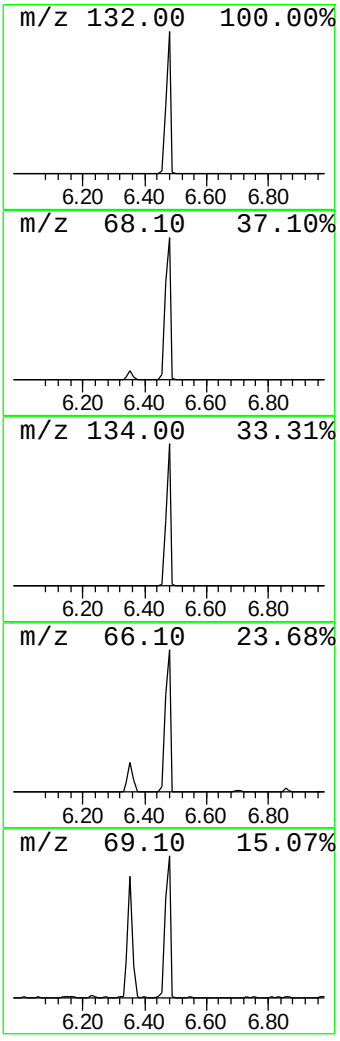
****

Peak Number 6 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	91.00 ng	1597070	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

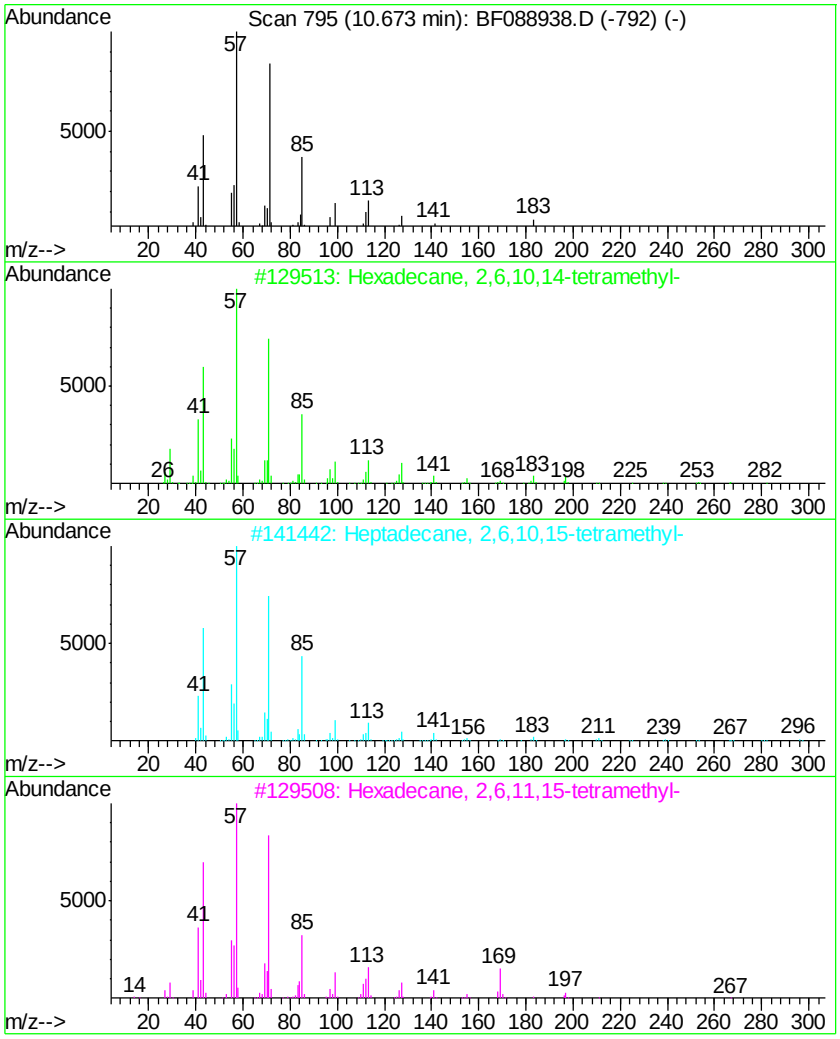
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

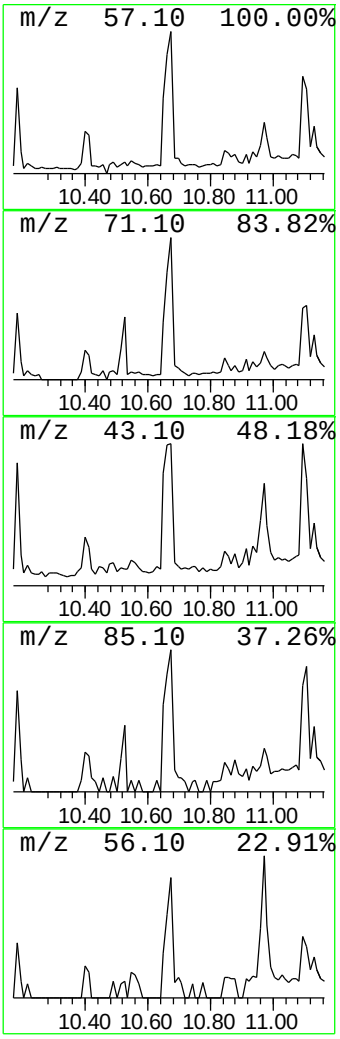
****

Peak Number 8 Hexadecane, 2,6,10,14-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	5.37 ng	94223	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	90
4	Heneicosane	296	C21H44	000629-94-7	80
5	Hexacosane	366	C26H54	000630-01-3	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

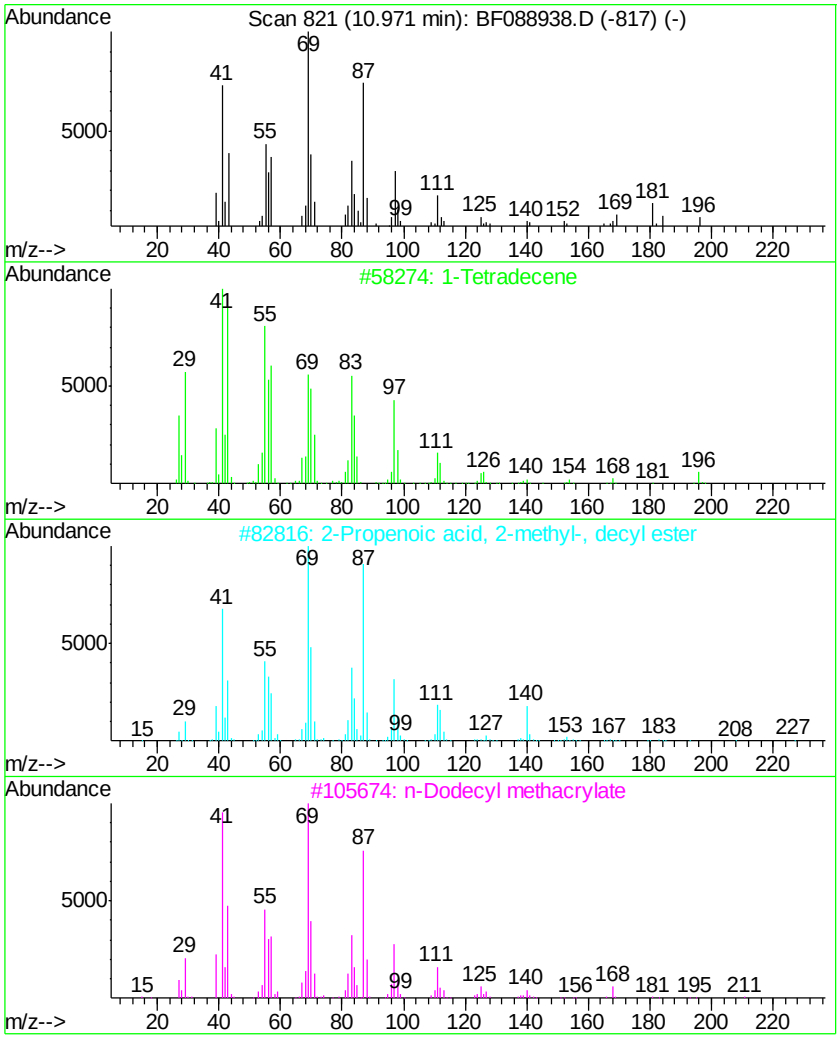
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

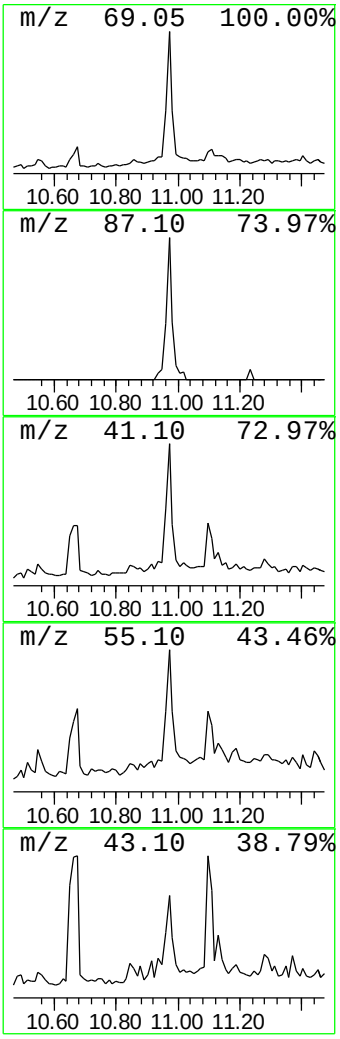
****

Peak Number 9 1-Tetradecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	7.11 ng	124801	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecene	196	C14H28	001120-36-1	90
2	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	90
3	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	90
4	Methacrylic acid, tetradecyl ester	282	C18H34O2	1000340-29-0	60
5	Cyclopropane, 1,1-dimethyl-2-nonyl-	196	C14H28	041977-38-2	60





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

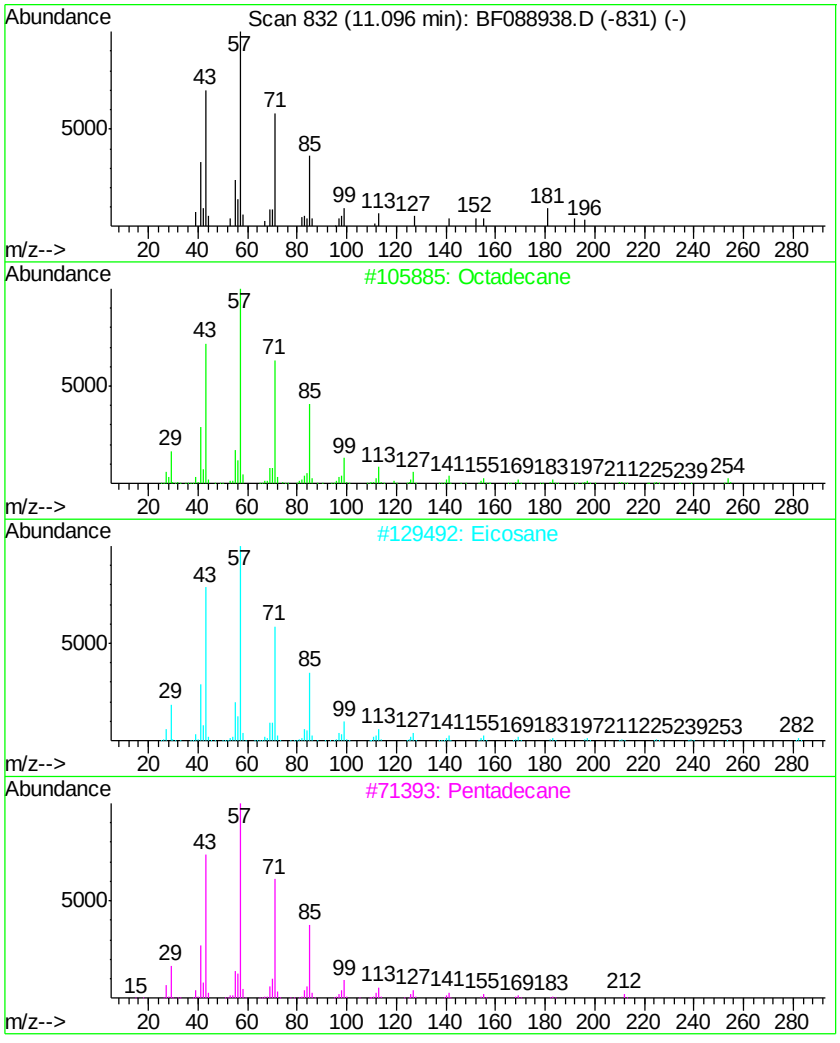
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

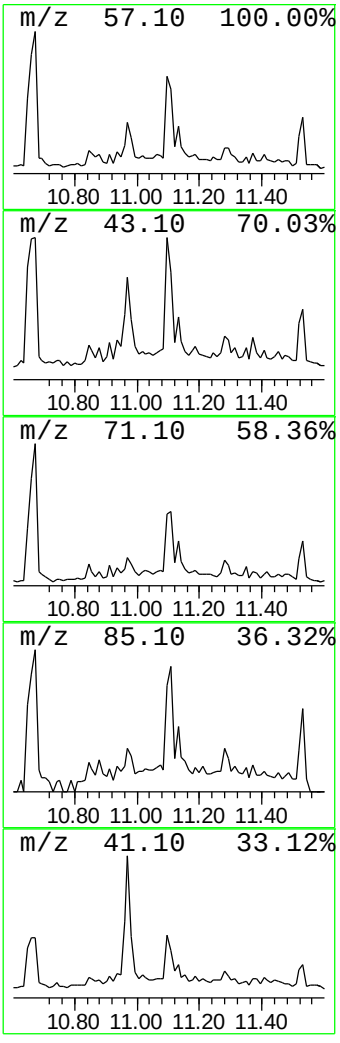
****

Peak Number 10 Octadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	2.62 ng	45964	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	72
2	Eicosane	282	C20H42	000112-95-8	72
3	Pentadecane	212	C15H32	000629-62-9	72
4	Tetratetracontane	619	C44H90	007098-22-8	72
5	Docosane	310	C22H46	000629-97-0	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

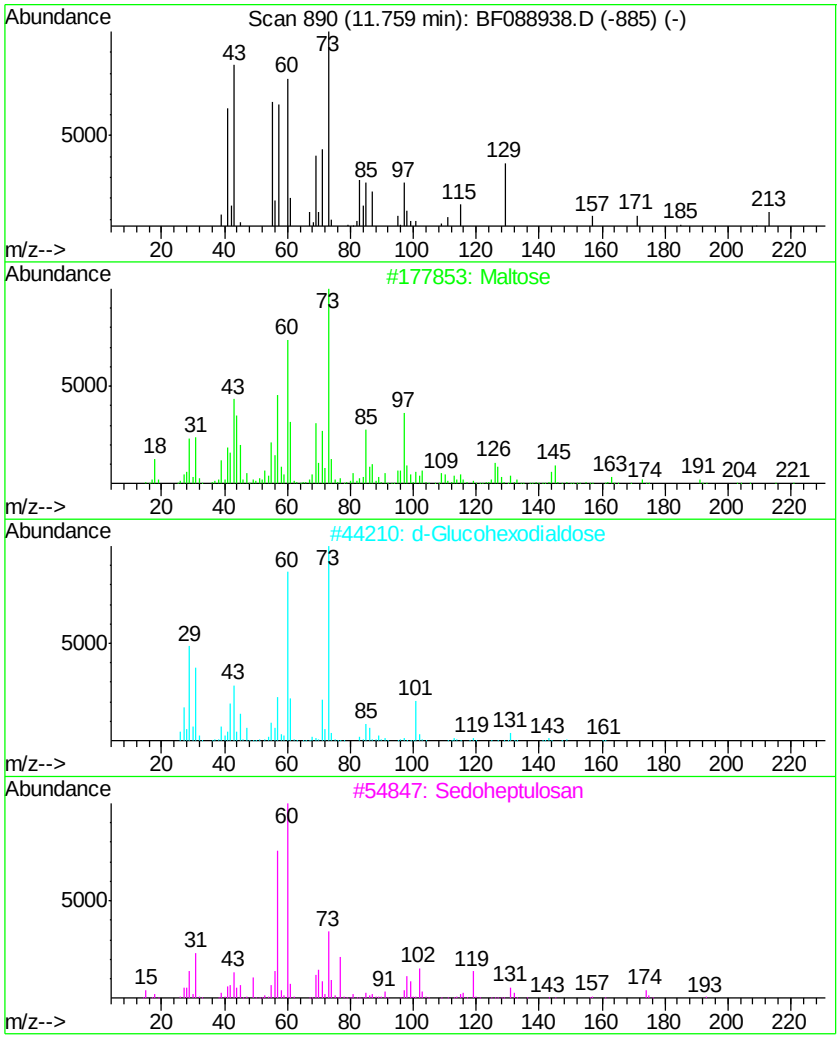
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

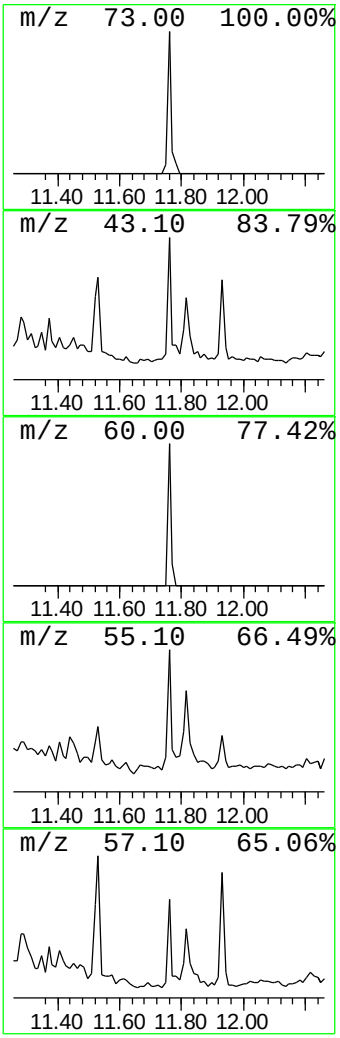
****

Peak Number 11 unknown11.76 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	4.25 ng	74669	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Maltose	342	C12H22O11	000069-79-4	43
2	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	38
3	Sedoheptulosan	192	C7H12O6	000469-90-9	27
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	18
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

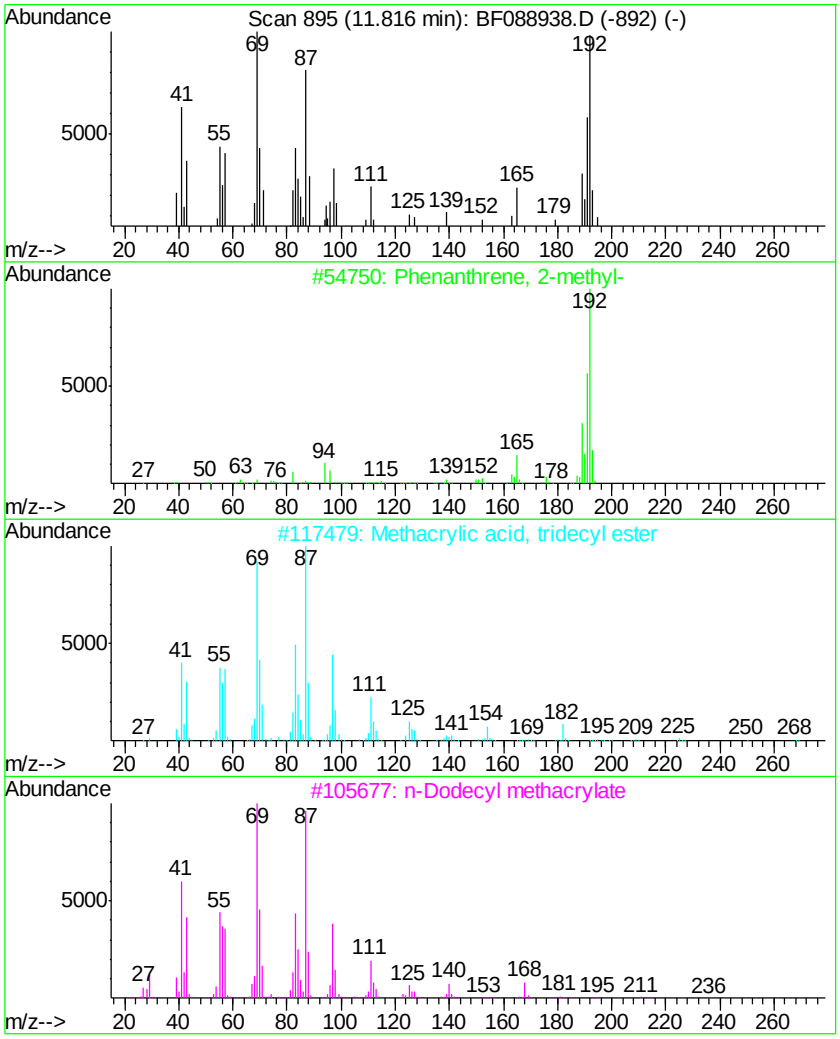
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

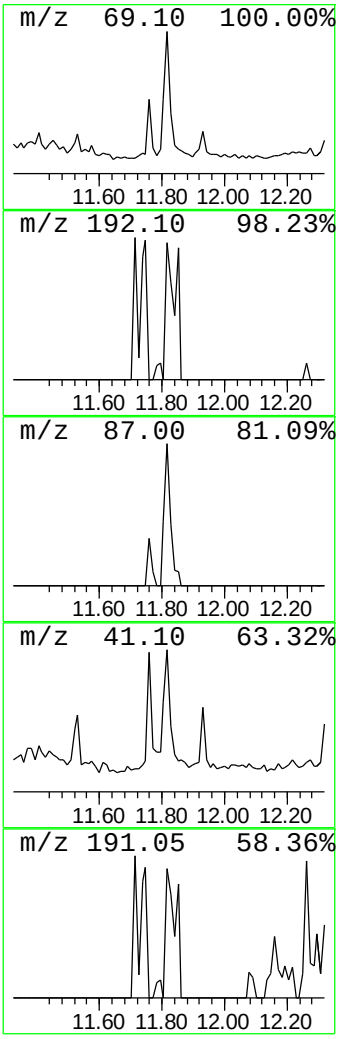
****

Peak Number 12 unknown11.82 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	4.62 ng	81173	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	46
2	Methacrylic acid, tridecyl ester	268	C17H32O2	1000340-28-9	45
3	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	45
4	Methacrylic acid, tetradecyl ester	282	C18H34O2	1000340-29-0	38
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

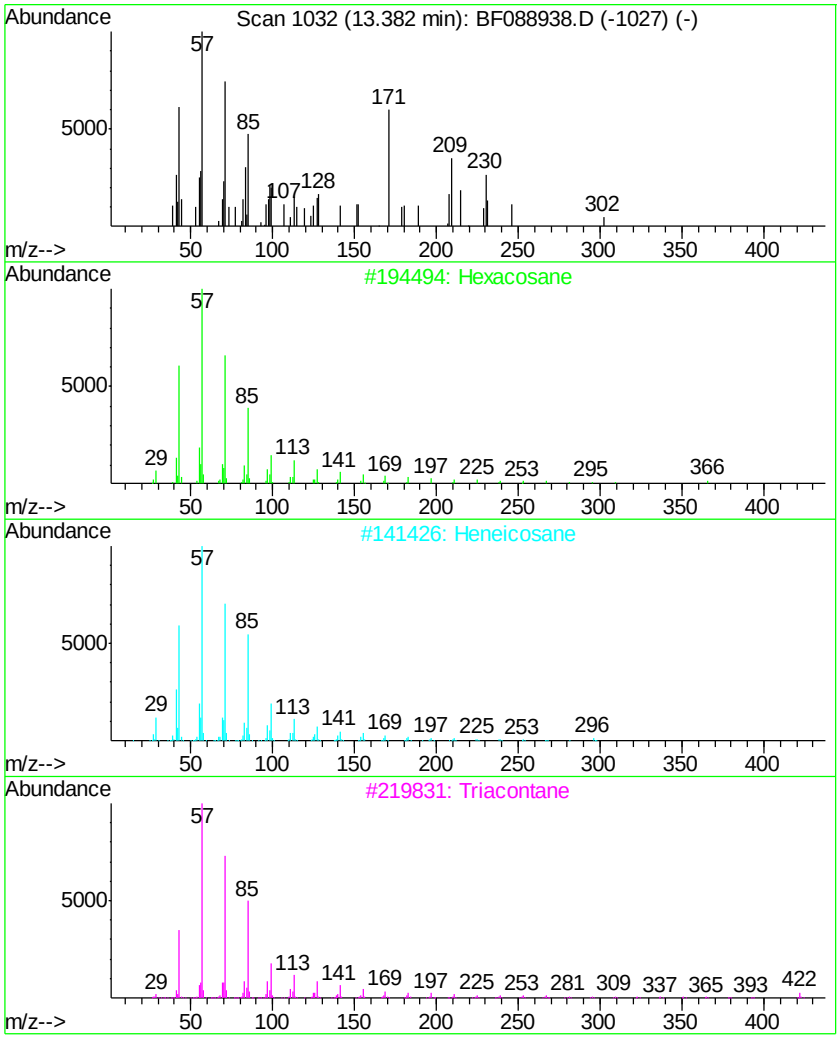
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

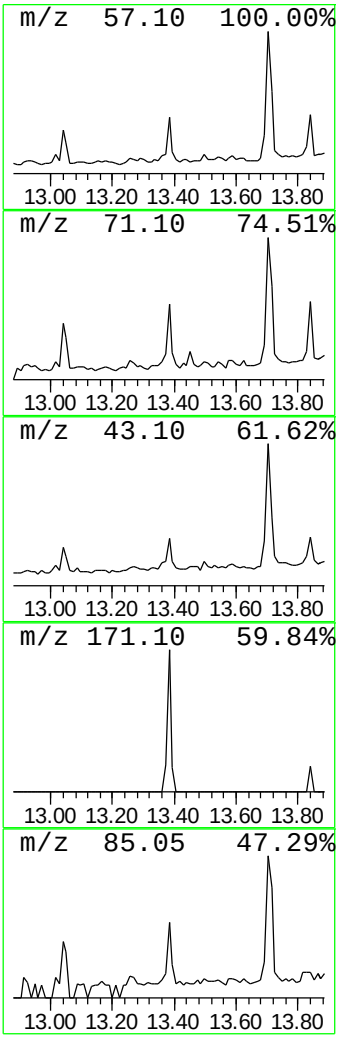
****

Peak Number 13 unknown13.38 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.38	2.39 ng	55653	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	46
2	Heneicosane	296	C21H44	000629-94-7	43
3	Triacontane	422	C30H62	000638-68-6	43
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	43
5	Pentacosane	352	C25H52	000629-99-2	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

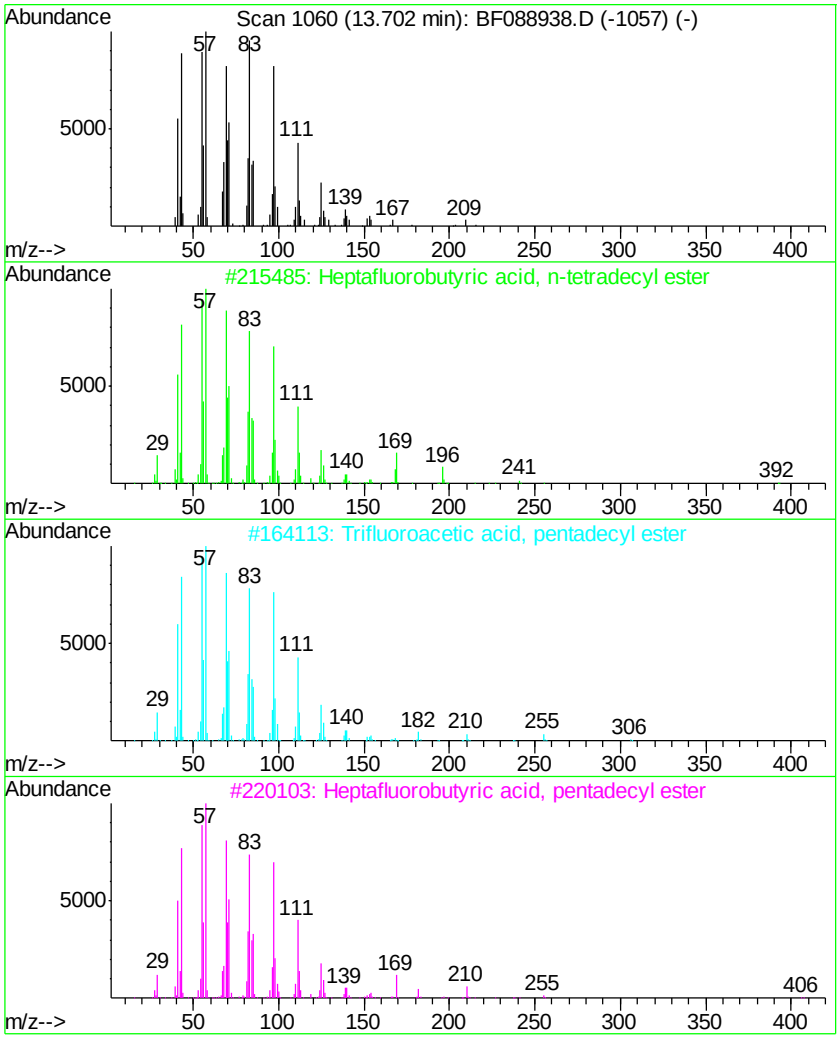
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

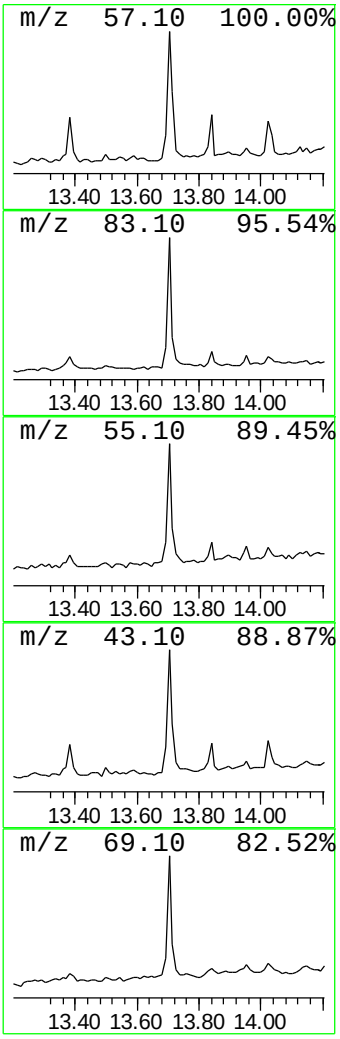
****

Peak Number 14 Heptafluorobutyric acid, n-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	5.37 ng	125047	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
4	1-Heneicosanol	312	C21H44O	015594-90-8	95
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	95





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

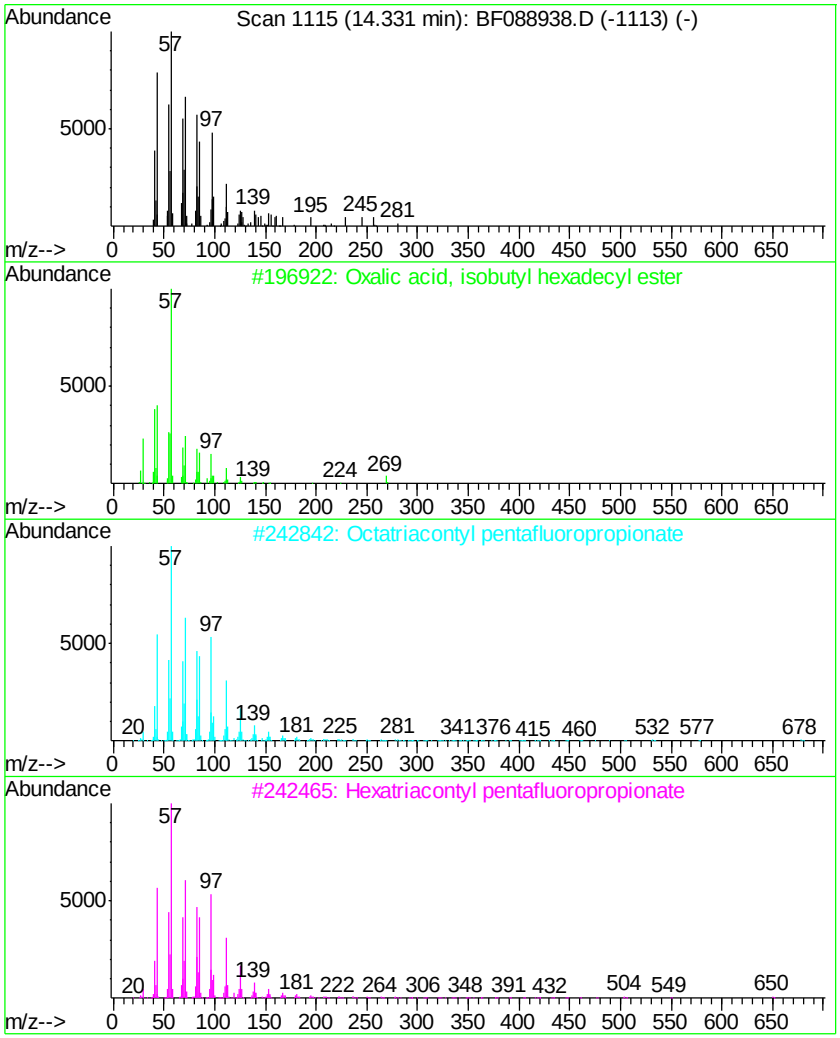
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

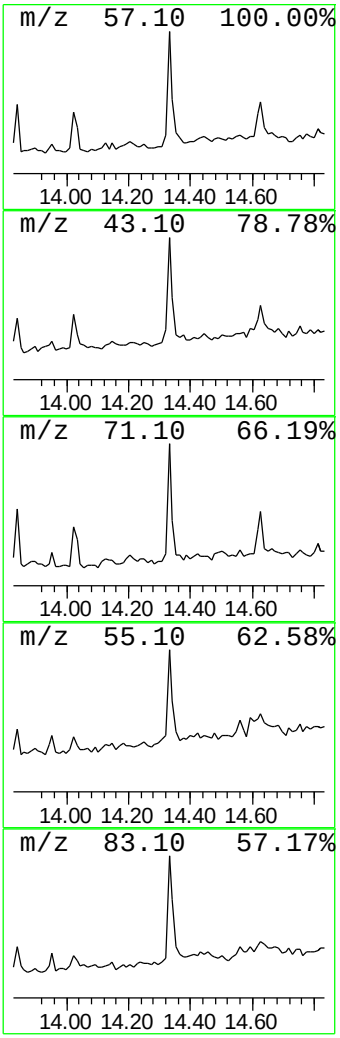
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Oxalic acid, isobutyl hexad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	4.32 ng	100558	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	87
3	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	87
4	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	83
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	83





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

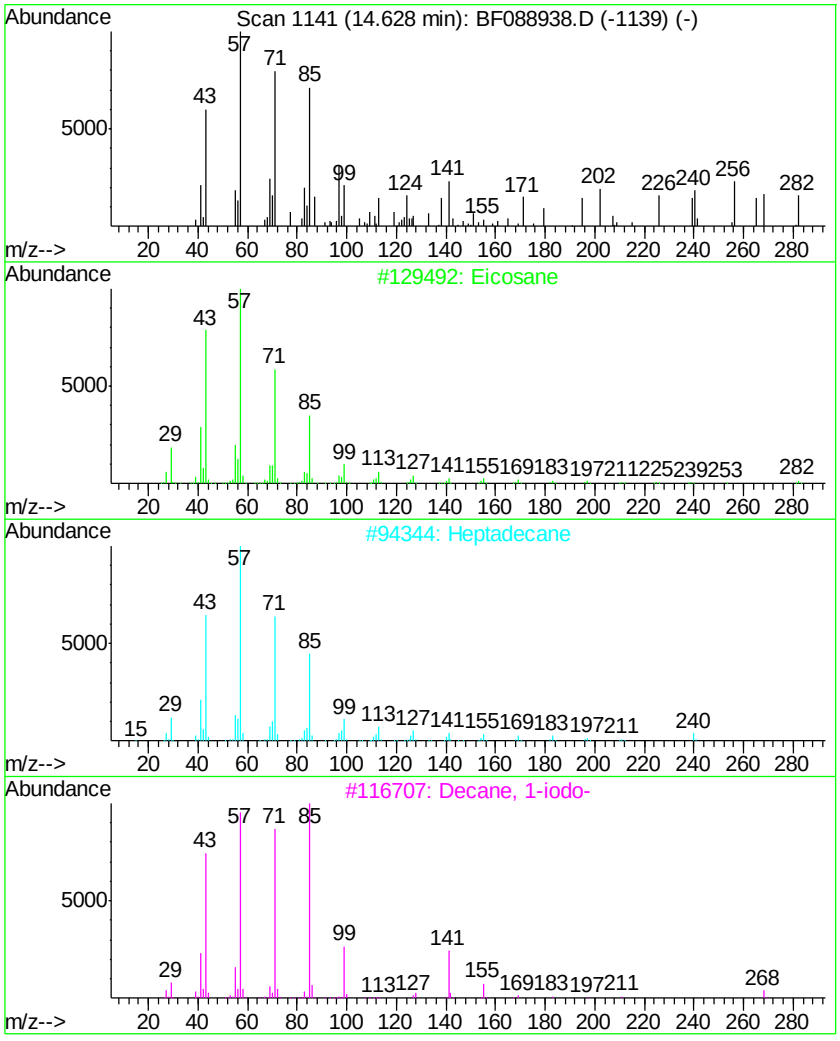
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

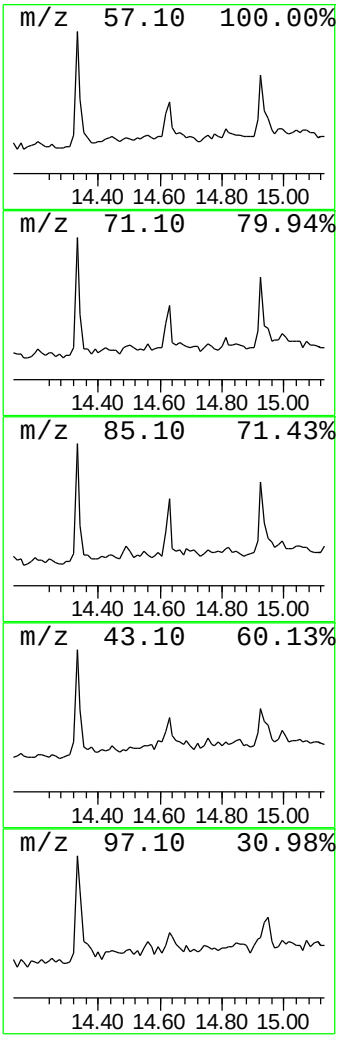
****

Peak Number 16 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.97 ng	46104	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	58
2	Heptadecane	240	C17H36	000629-78-7	58
3	Decane, 1-iodo-	268	C10H21I	002050-77-3	58
4	Nonadecane	268	C19H40	000629-92-5	58
5	Hexadecane	226	C16H34	000544-76-3	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

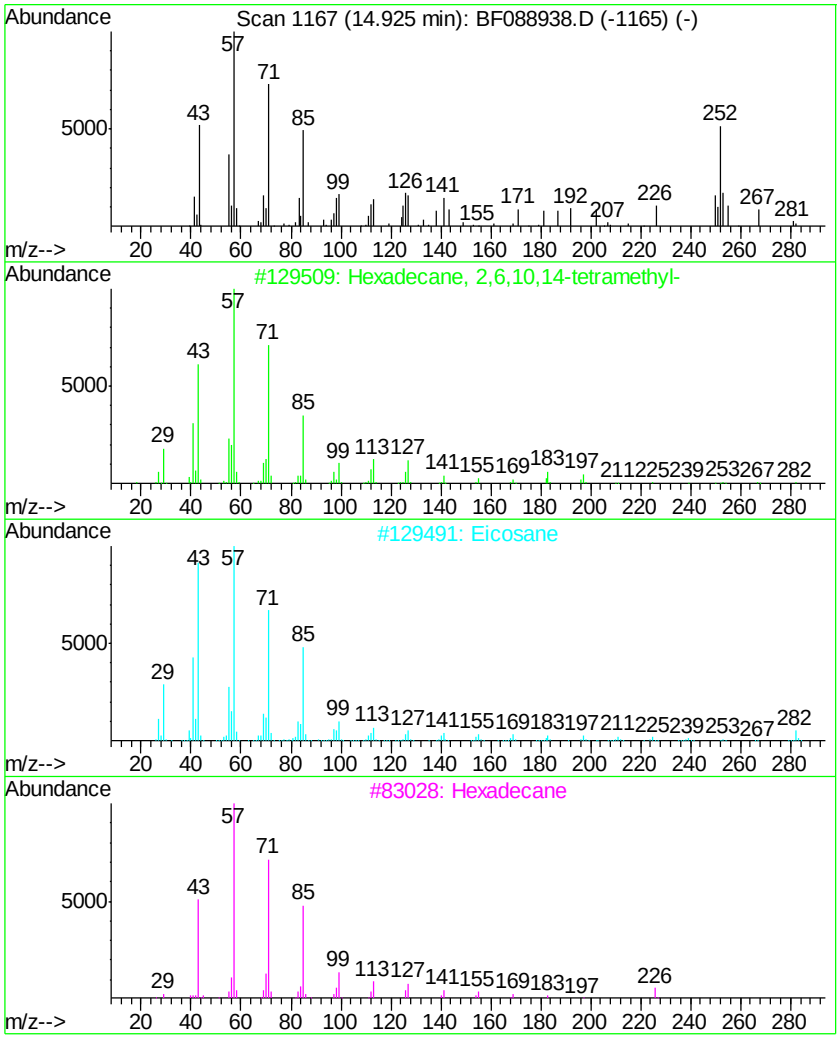
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

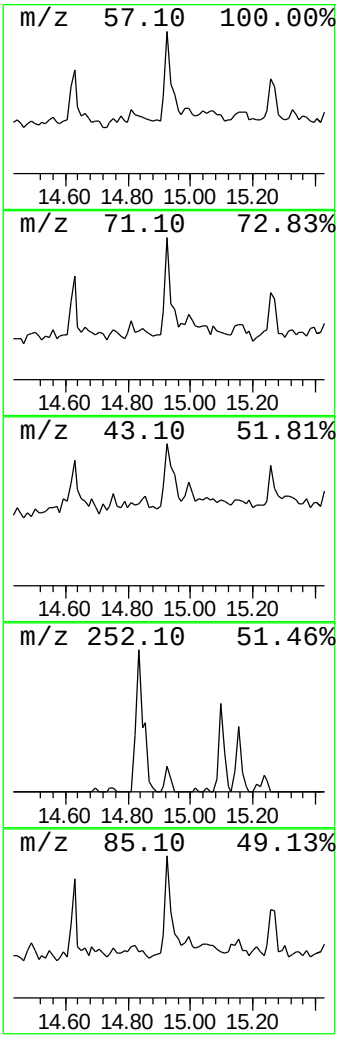
****

Peak Number 17 unknown14.93 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.45 ng	38014	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	46
2	Eicosane	282	C20H42	000112-95-8	46
3	Hexadecane	226	C16H34	000544-76-3	43
4	Heneicosane	296	C21H44	000629-94-7	38
5	Decane, 5-propyl-	184	C13H28	017312-62-8	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

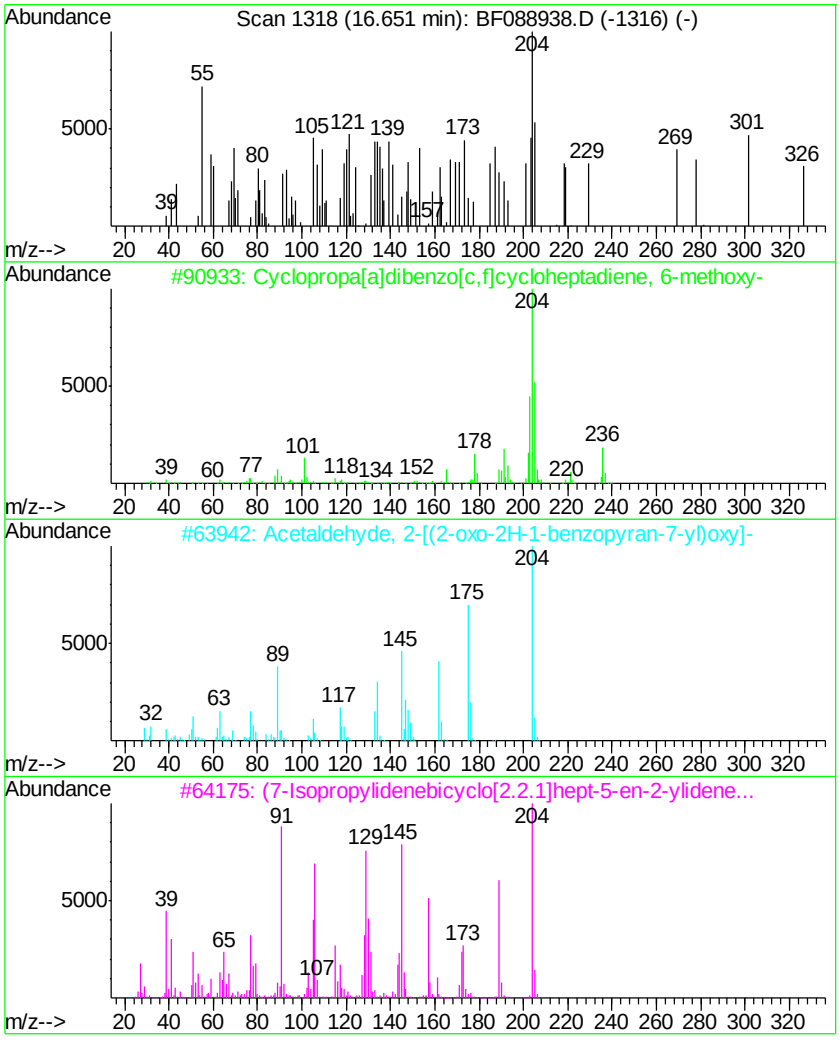
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

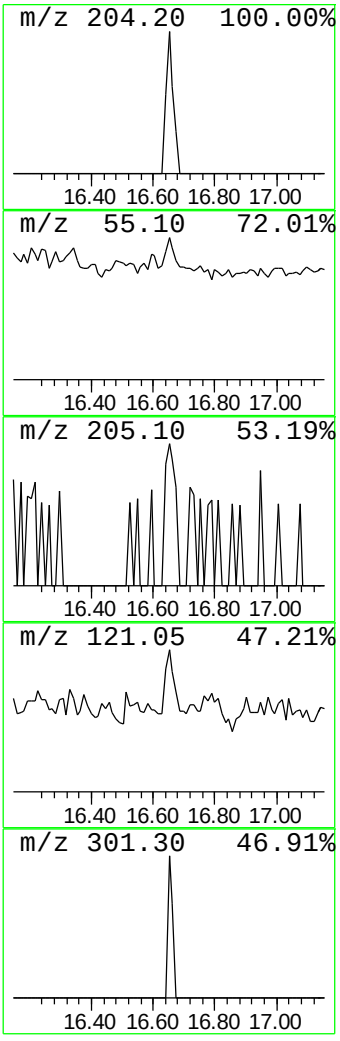
****

Peak Number 19 unknown16.65 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.65	2.59 ng	40262	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropa[a]dibenzo[c,f]cyclohe...	236	C17H16O	1000210-38-0	27
2	Acetaldehyde, 2-[(2-oxo-2H-1-ben...	204	C11H8O4	1000319-48-8	11
3	(7-Isopropylidenebicyclo[2.2.1]h...	204	C13H16O2	1000211-02-2	11
4	1H-1,2-Azaphosphole, 1-(1,1-dime...	219	C13H18NP	071236-84-5	10
5	3,5-Dichloro-2,4-dimethyl-1-meth...	204	C9H10Cl2O	1000250-17-8	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

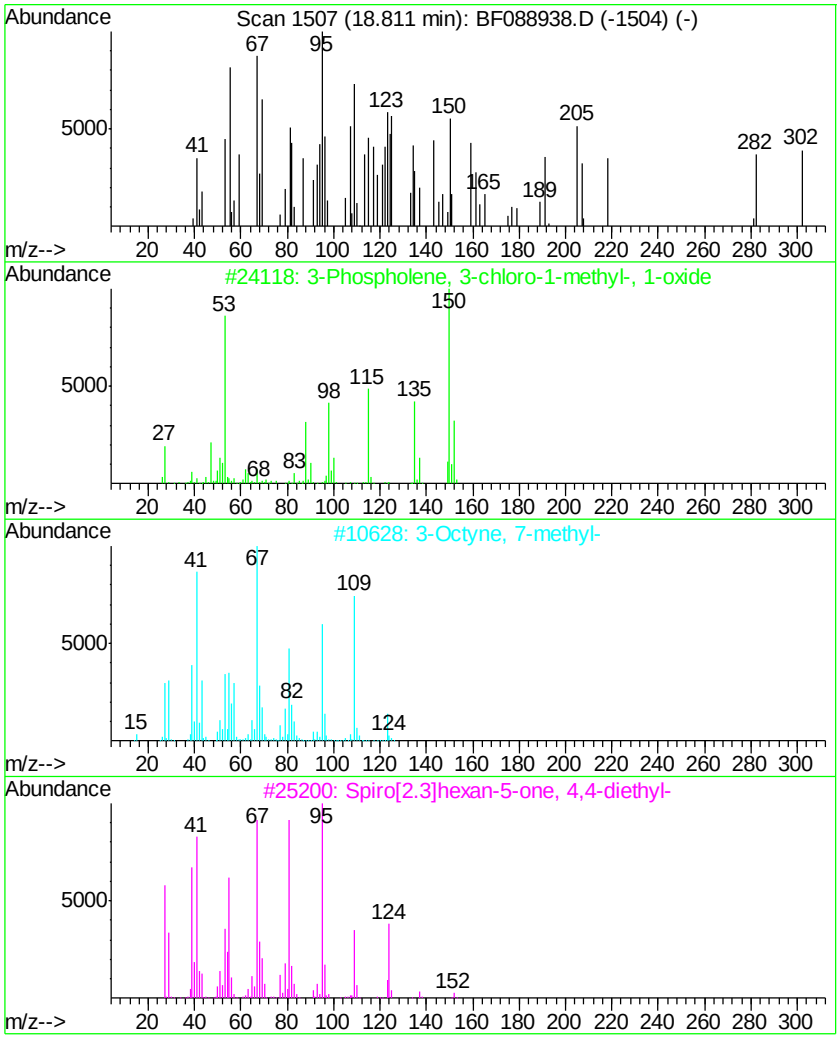
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

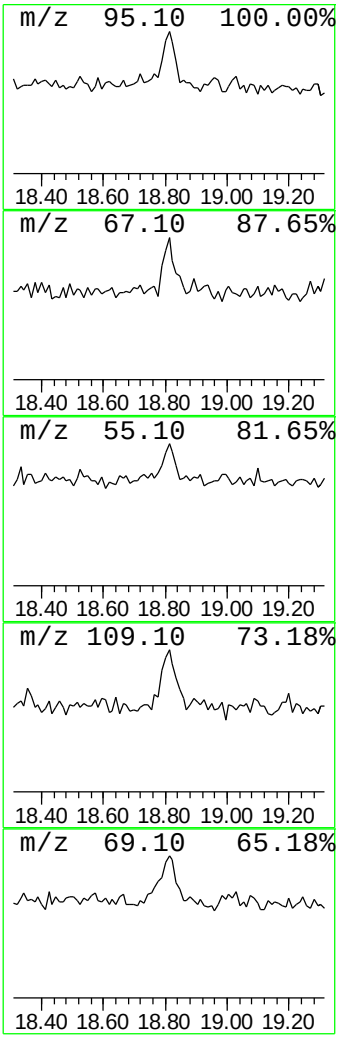
****

Peak Number 20 unknown18.81 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.81	3.66 ng	56811	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phospholene, 3-chloro-1-methyl...	150	C5H8ClOP	022356-34-9	25
2	3-Octyne, 7-methyl-	124	C9H16	037050-06-9	25
3	Spiro[2.3]hexan-5-one, 4,4-diethyl-	152	C10H16O	1000154-16-2	25
4	3-Octyne	110	C8H14	015232-76-5	14
5	8-Thiabicyclo[4.3.0]nonane S-oxide	158	C8H14OS	1000215-10-0	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088938.D
Acq On : 13 Jul 2016 00:25
Operator : UM/SJ
Sample : H3935-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C3-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	1.88	4.4	ng	76982	1	6.71	350986	20.0
R-(-)-1,2-propane...	2.87	2.9	ng	50099	1	6.71	350986	20.0
2-Pentanone, 4-hy...	4.86	11.1	ng	194805	1	6.71	350986	20.0
unknown6.48	6.48	91.0	ng	1597070	1	6.71	350986	20.0
Hexadecane, 2,6,1...	10.67	5.4	ng	94223	4	11.21	351096	20.0
1-Tetradecene	10.97	7.1	ng	124801	4	11.21	351096	20.0
Octadecane	11.10	2.6	ng	45964	4	11.21	351096	20.0
unknown11.76	11.76	4.3	ng	74669	4	11.21	351096	20.0
unknown11.82	11.82	4.6	ng	81173	4	11.21	351096	20.0
unknown13.38	13.38	2.4	ng	55653	5	13.84	465824	20.0
Heptafluorobutyri...	13.70	5.4	ng	125047	5	13.84	465824	20.0
Oxalic acid, isob...	14.33	4.3	ng	100558	5	13.84	465824	20.0
Eicosane	14.63	3.0	ng	46104	6	15.21	310696	20.0
unknown14.93	14.93	2.5	ng	38014	6	15.21	310696	20.0
unknown16.65	16.65	2.6	ng	40262	6	15.21	310696	20.0
unknown18.81	18.81	3.7	ng	56811	6	15.21	310696	20.0