LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073018\
Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-21

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.154	133	139	145	rBV	76060	132526	2.60%	0.392%
2	5.189	482	485	492	rBV	231794	269565	5.30%	0.797%
3	5.601	551	555	569	rBV	1006561	1653356	32.48%	4.890%
4	6.119	640	643	649	rVB2	41388	54746	1.08%	0.162%
5	6.548	712	716	722	rVB4	59422	65737	1.29%	0.194%
6	6.607	722	726	744	rBV	465872	1293473	25.41%	3.826%
7	6.736	744	748	768	rVV	2993504	3859106	75.82%	11.414%
8	6.966	783	787	793	rVV	598385	857722	16.85%	2.537%
9	7.013	793	795	806	rVV2	142434	235286	4.62%	0.696%
10	7.119	809	813	824	rVV	3285064	3732000	73.32%	11.038%
11	7.195	824	826	836	rVV3	109253	247955	4.87%	0.733%
12	7.289	840	842	849	rVV	73122	80789	1.59%	0.239%
13	7.348	849	852	858	rVB4	60216	68742	1.35%	0.203%
14	7.489	869	876	879	rBV	123373	145457	2.86%	0.430%
15	7.531	879	883	892	rBV	1961103	2681820	52.69%	7.932%
16	7.883	939	943	947	rBV3	73478	100551	1.98%	0.297%
17	7.978	954	959	961	rBV	182551	193817	3.81%	0.573%
18	8.248	1001	1005	1015	rBV2	876583	1357423	26.67%	4.015%
19	8.483	1041	1045	1049	rBV3	58427	74110	1.46%	0.219%
20	9.060	1139	1143	1145	rBV	91286	89244	1.75%	0.264%
21	9.319	1181	1187	1203	rBV	4189296	5089870	100.00%	15.054%
22	9.654	1241	1244	1249	rVV2	91176	91782	1.80%	0.271%
23	9.707	1249	1253	1260	rVB	214027	236864	4.65%	0.701%
24	10.001	1296	1303	1308	rBV	1139060	1266150	24.88%	3.745%
25	10.801	1435	1439	1451	rBV	2041666	2666202	52.38%	7.886%
26	10.930	1458	1461	1467	rVB	52707	74377	1.46%	0.220%
27	11.501	1554	1558	1577	rBV	819149	1074159	21.10%	3.177%
28	12.007	1640	1644	1648	rBV	114745	144281	2.83%	0.427%
29	12.954	1803	1805	1808	rBV3	44581	54818	1.08%	0.162%
30	13.083	1823	1827	1836	rBV	3345772	3751435	73.70%	11.095%
31	13.954	1973	1975	1982	rVB	211645	284021	5.58%	0.840%
32	14.154	2006	2009	2015	rBV	822389	956590	18.79%	2.829%
33	14.977	2147	2149	2152	rBV	275272	290704	5.71%	0.860%
34	15.689	2267	2270	2278	rBV2	395027	636081	12.50%	1.881%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073018\
Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-21

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 33810759

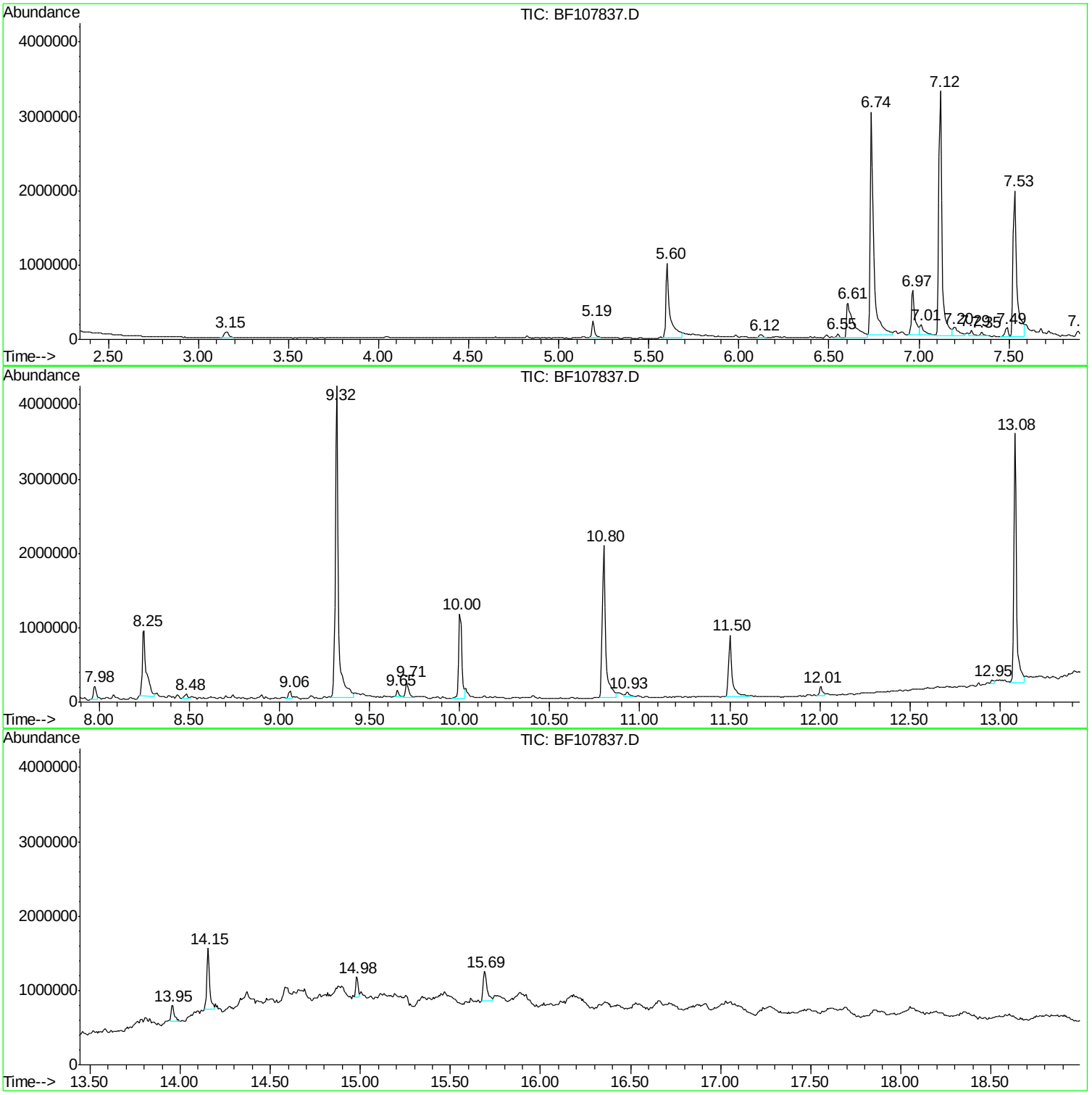
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073018\
Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073018\
Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

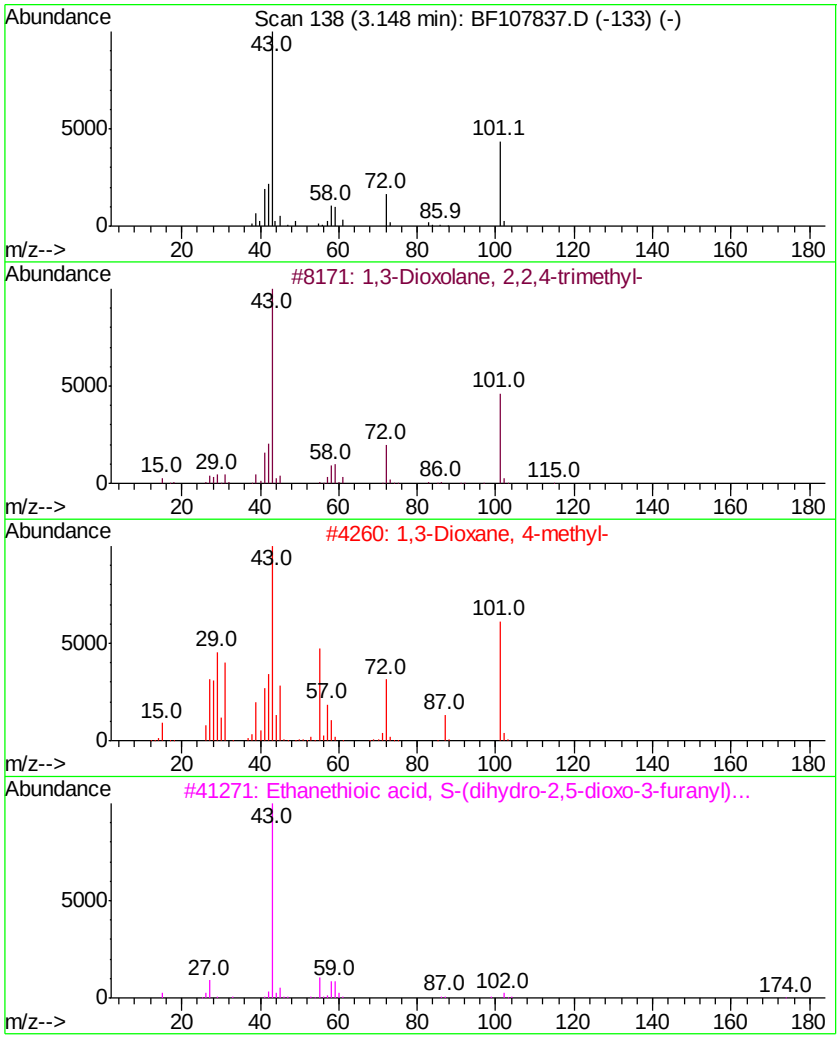
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

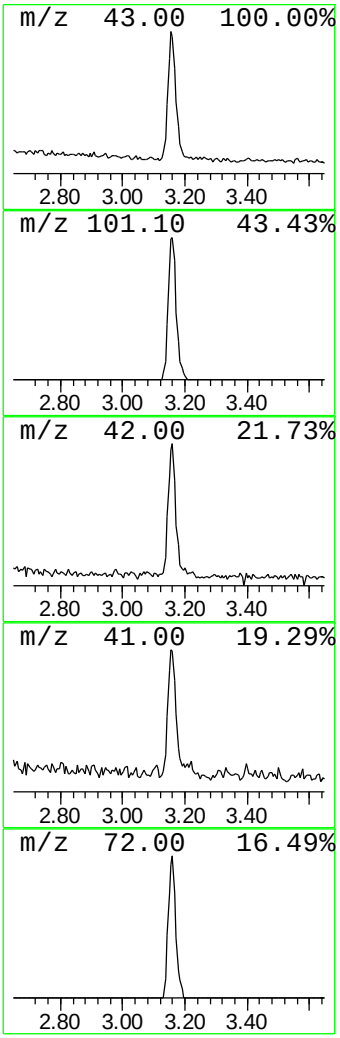
****

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	3.09 ng	132526	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	45
3	Ethanethioic acid, S-(dihydro-2,...	174	C6H6O4S	006953-60-2	10
4	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
5	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073018\
Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

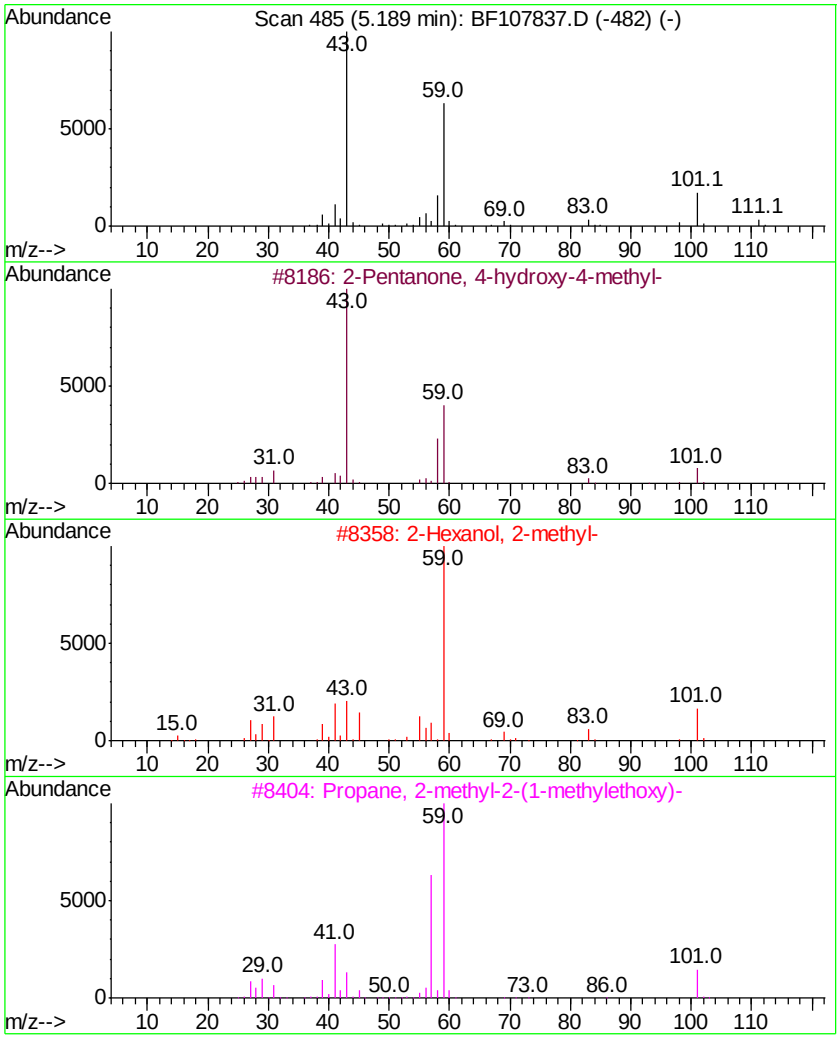
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

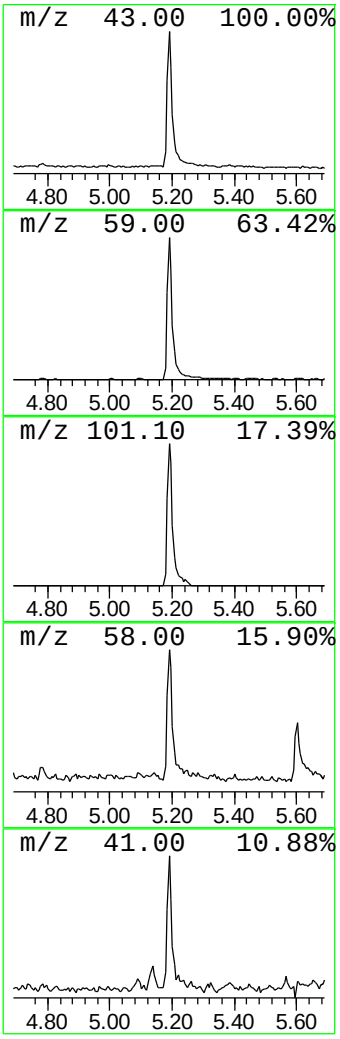
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	6.29 ng	269565	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	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	47
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	37
5	3-Octanol	130	C8H18O	000589-98-0	36





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073018\
Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

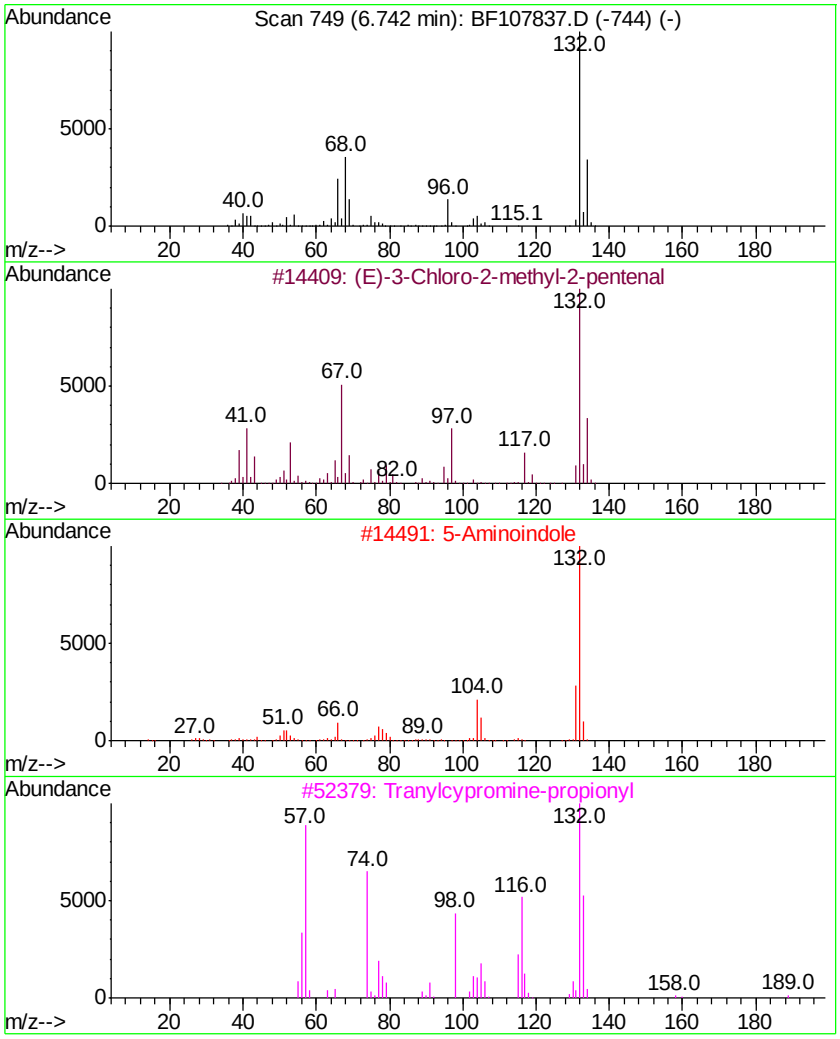
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

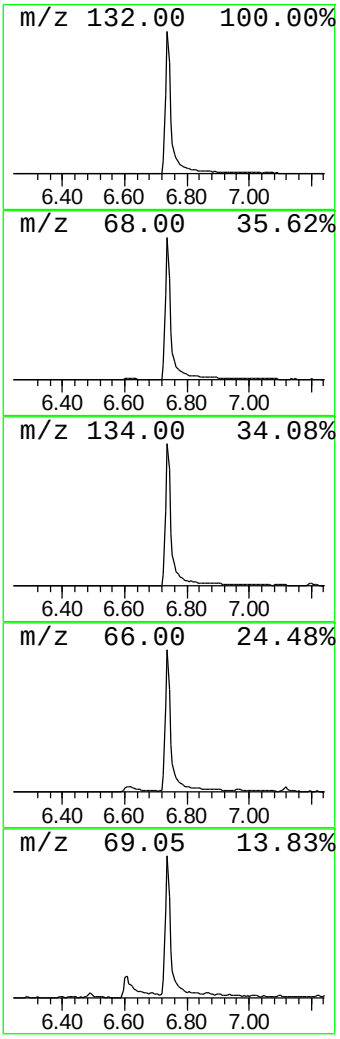
****

Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	89.99 ng	3859110	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073018\
Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

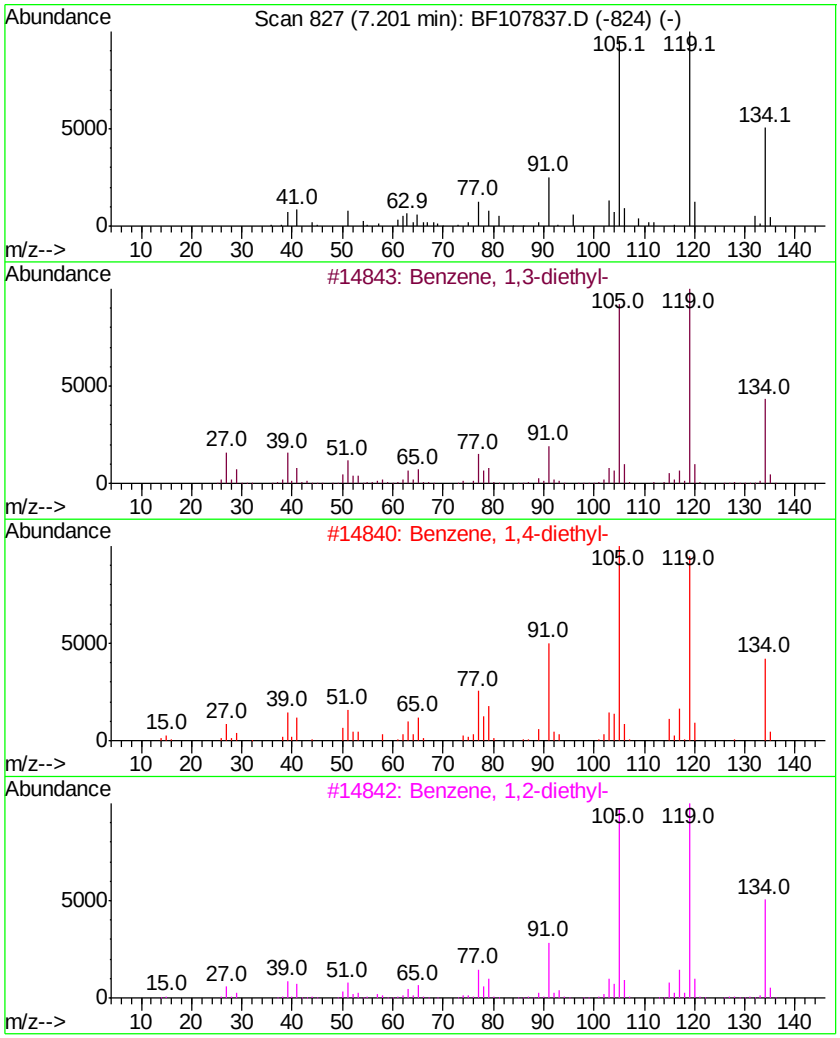
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

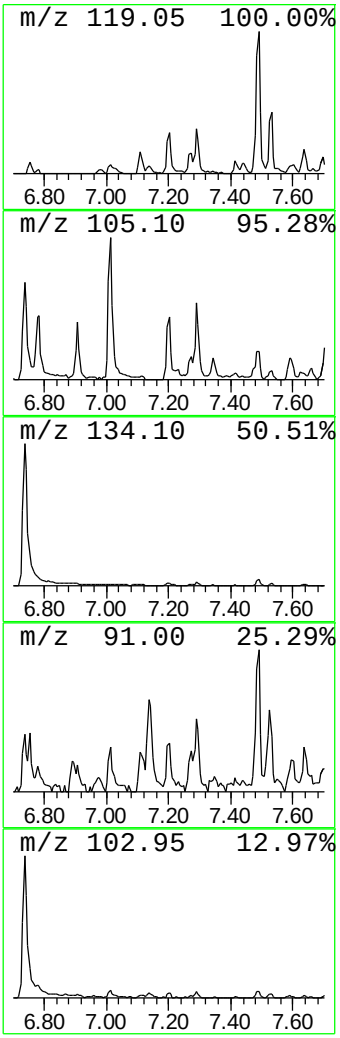
****

Peak Number 5 Benzene, 1,3-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	5.78 ng	247955	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	91
2	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	91
3	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	91
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	86
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073018\
Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

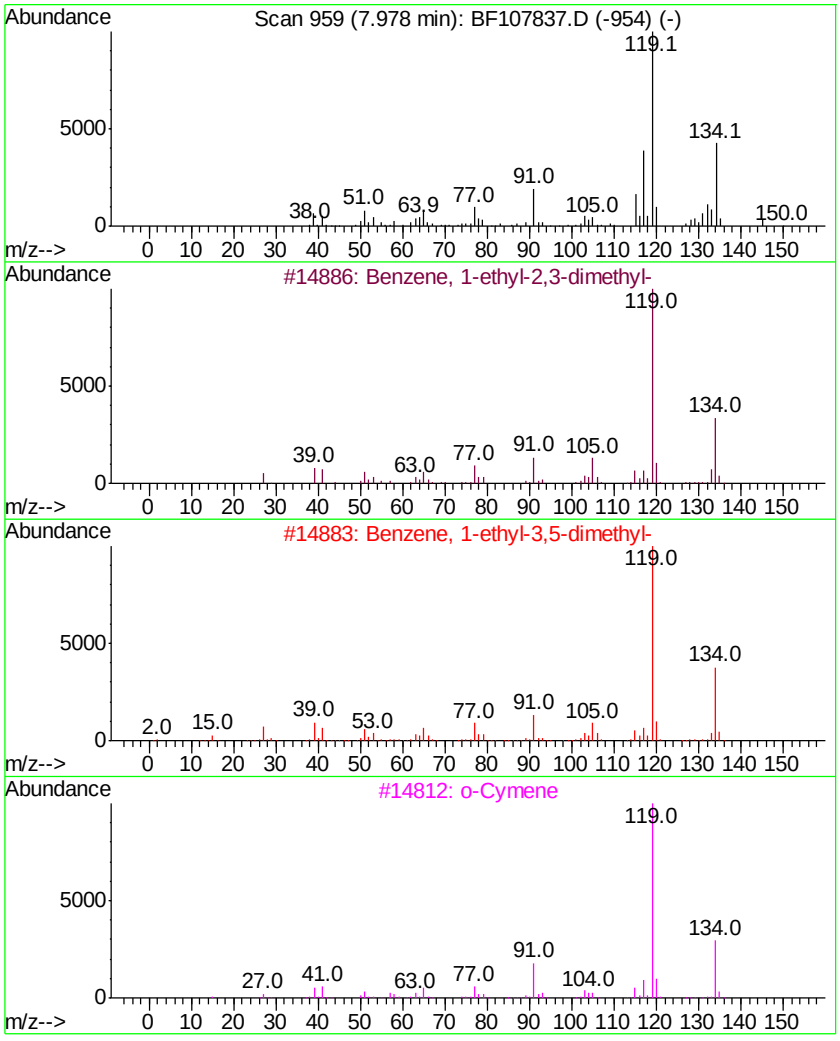
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

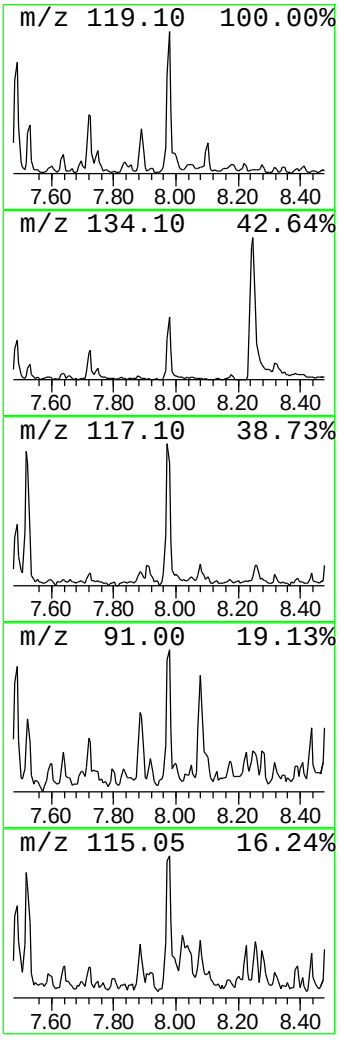
****

Peak Number 6 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.98	2.86 ng	193817	Naphthalene-d8	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	70
2	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	70
3	o-Cymene	134	C10H14	000527-84-4	70
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	70
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	70





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073018\
Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

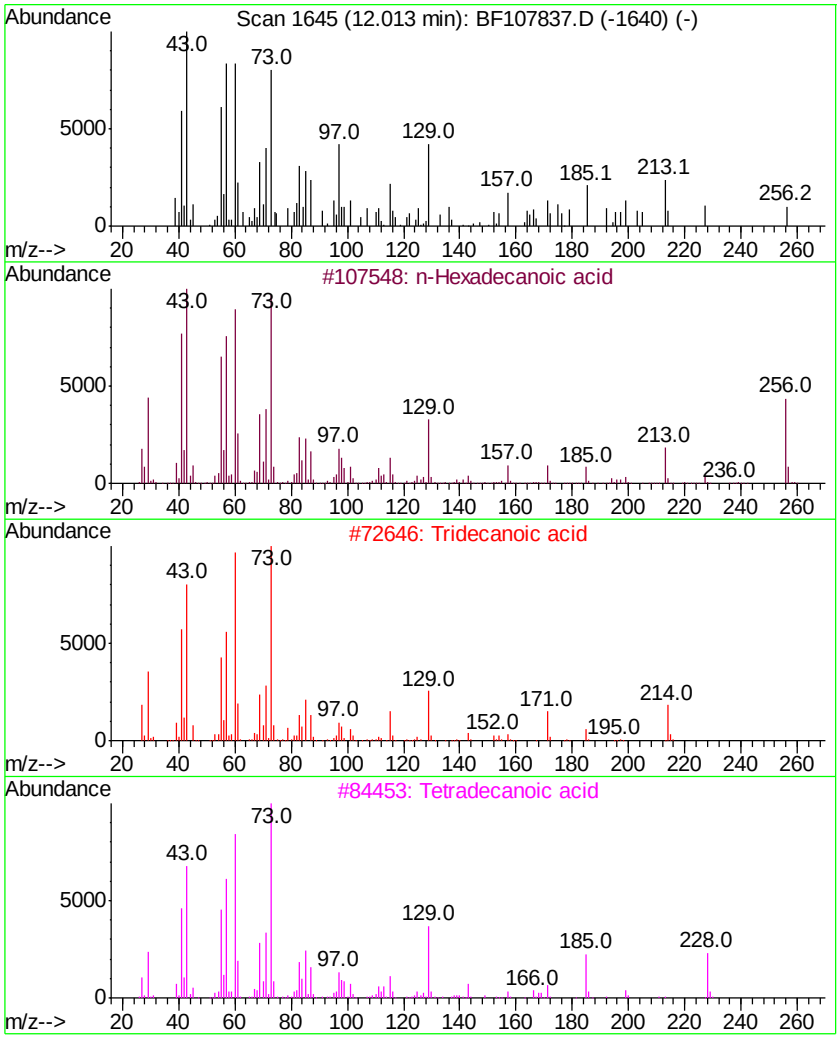
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

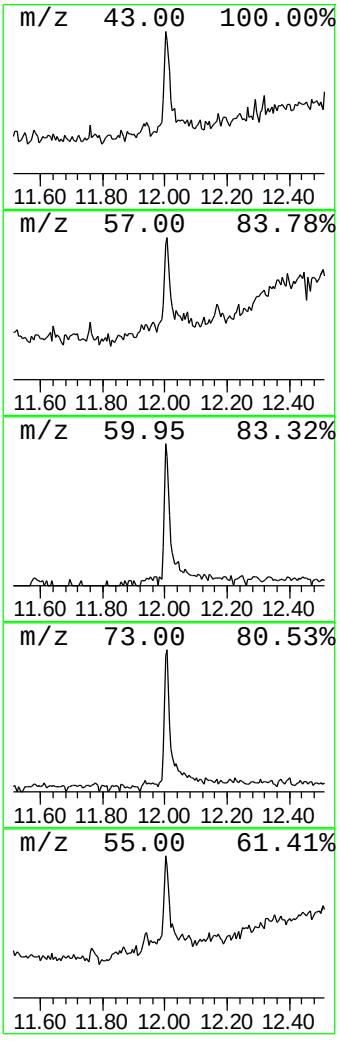
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.69 ng	144281	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	62





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Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

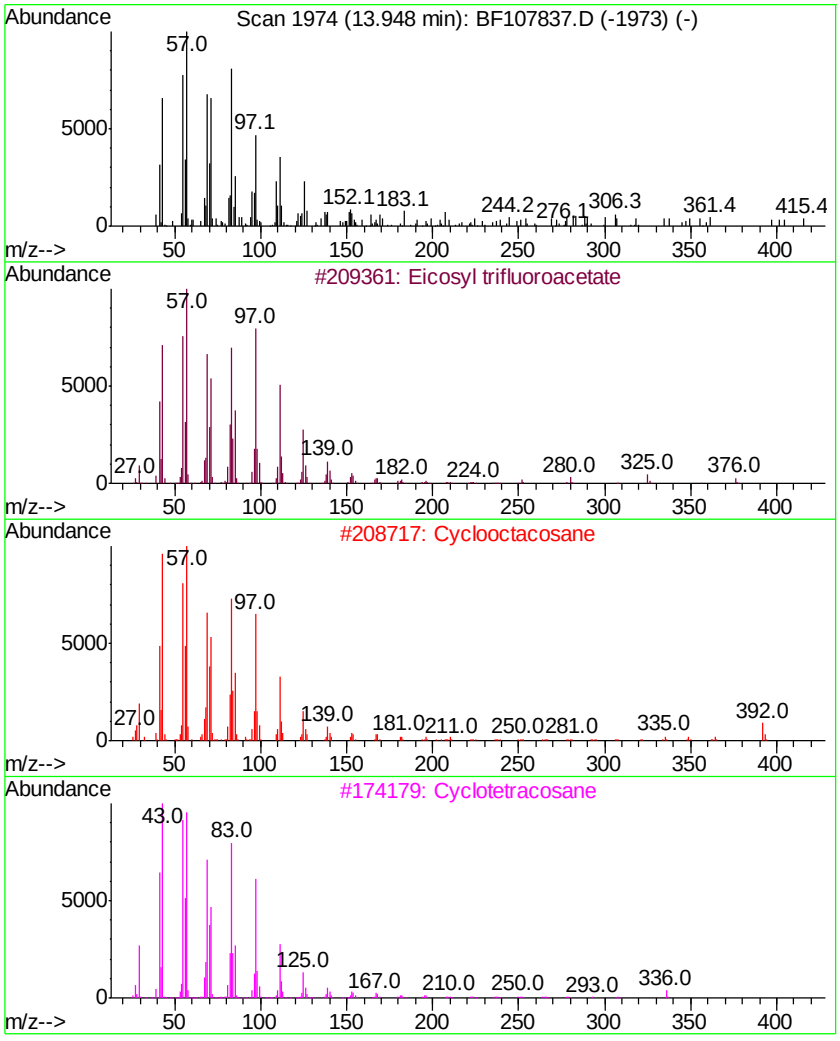
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

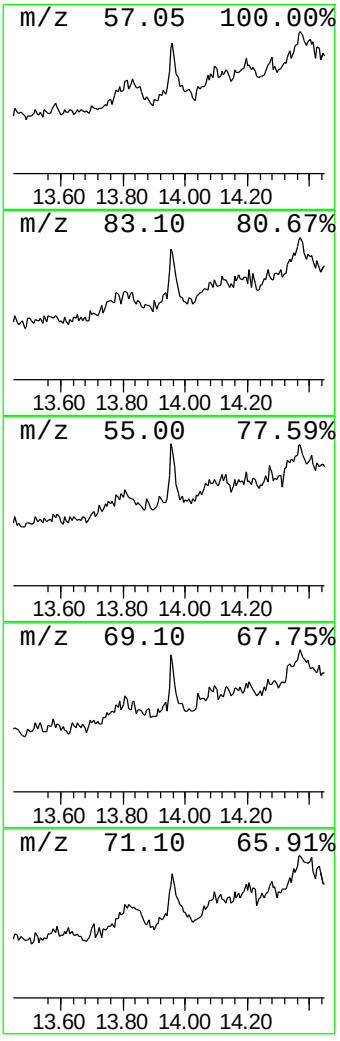
****

Peak Number 8 Eicosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	5.94 ng	284021	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	87
2	Cyclooctacosane	392	C28H56	000297-24-5	87
3	Cyclotetracosane	336	C24H48	000297-03-0	83
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	83
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83





Library Search Compound Report

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Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

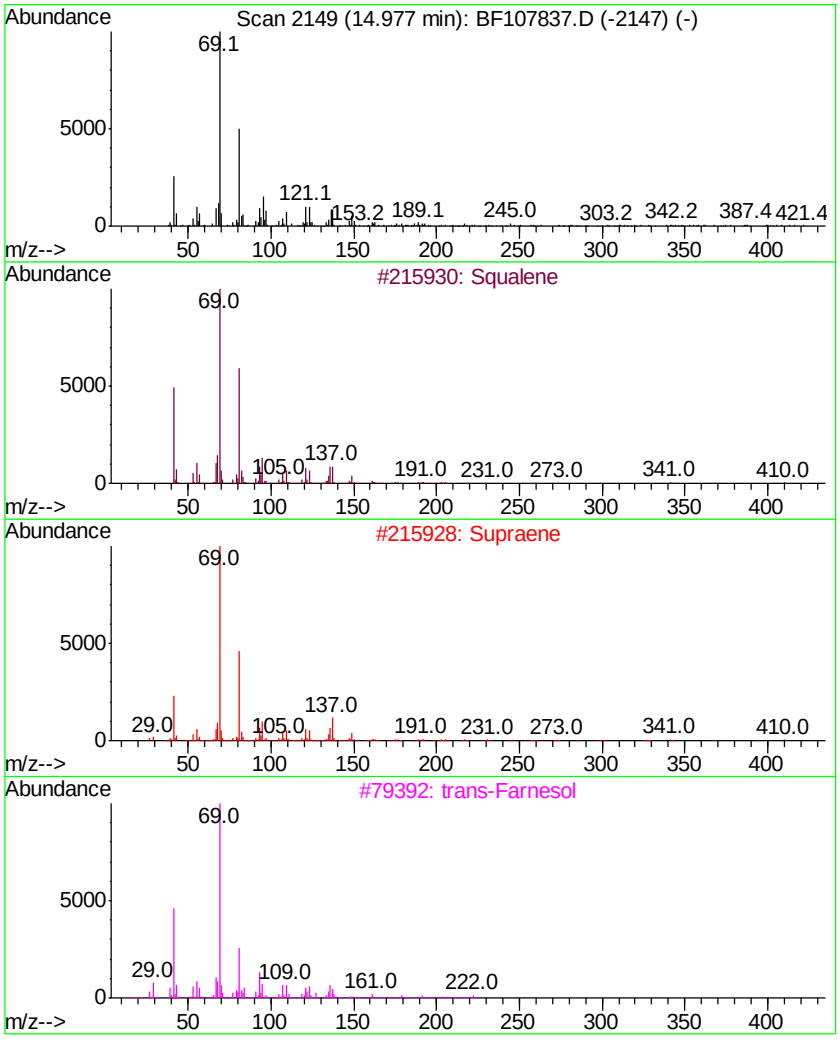
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

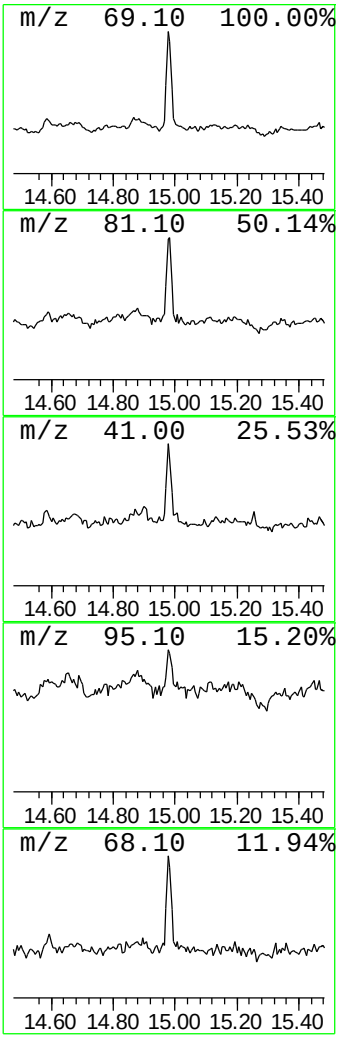
****

Peak Number 9 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	9.14 ng	290704	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	74
3	trans-Farnesol	222	C15H26O	000106-28-5	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-69-1	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF073018\
Data File : BF107837.D
Acq On : 31 Jul 2018 8:25
Operator : JU/SJ
Sample : J4221-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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
1,3-Dioxolane, 2,...	3.15	3.1	ng	132526	1	6.97	857722	20.0
2-Pentanone, 4-hy...	5.19	6.3	ng	269565	1	6.97	857722	20.0
unknown6.74	6.74	90.0	ng	3859110	1	6.97	857722	20.0
Benzene, 1,3-diet...	7.20	5.8	ng	247955	1	6.97	857722	20.0
Benzene, 1-ethyl-...	7.98	2.9	ng	193817	2	8.25	1357420	20.0
n-Hexadecanoic acid	12.01	2.7	ng	144281	4	11.50	1074160	20.0
Eicosyl trifluoro...	13.95	5.9	ng	284021	5	14.15	956590	20.0
Squalene	14.98	9.1	ng	290704	6	15.69	636081	20.0