LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092618\
Data File : BF109338.D
Acq On : 26 Sep 2018 16:01
Operator : JU/SJ
Sample : J5070-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200027

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-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	473	477	486	rVB	45011	55893	3.68%	0.353%
2	5.310	544	548	552	rBV	1423329	1363336	89.69%	8.601%
3	5.957	652	658	661	rBV	301793	393366	25.88%	2.482%
4	6.340	719	723	733	rBV	1461855	1520045	100.00%	9.590%
5	6.475	742	746	749	rBV	1787583	1484963	97.69%	9.368%
6	6.545	755	758	762	rBV	18293	17837	1.17%	0.113%
7	6.704	782	785	789	rBV	720024	608062	40.00%	3.836%
8	6.863	808	812	815	rBV	1300102	1016702	66.89%	6.414%
9	7.263	876	880	883	rBV	1007800	881048	57.96%	5.558%
10	7.987	999	1003	1007	rBV	980098	780928	51.38%	4.927%
11	9.063	1182	1186	1189	rBV	1780631	1392242	91.59%	8.784%
12	9.186	1205	1207	1215	rVB	52853	49146	3.23%	0.310%
13	9.457	1249	1253	1256	rBV	492550	380369	25.02%	2.400%
14	9.739	1297	1301	1304	rBV	1044344	922945	60.72%	5.823%
15	10.328	1398	1401	1406	rVB	202168	163746	10.77%	1.033%
16	10.522	1430	1434	1440	rBV	1238054	1067437	70.22%	6.734%
17	11.216	1548	1552	1554	rBV	1104276	920210	60.54%	5.806%
18	11.233	1554	1555	1559	rVB	62135	48558	3.19%	0.306%
19	11.363	1573	1577	1581	rBV5	9834	19000	1.25%	0.120%
20	11.751	1640	1643	1653	rBV3	79518	112726	7.42%	0.711%
21	11.827	1653	1656	1659	rBV2	19398	32348	2.13%	0.204%
22	12.316	1737	1739	1742	rBV3	26908	29772	1.96%	0.188%
23	12.645	1793	1795	1797	rVB	50619	37795	2.49%	0.238%
24	12.792	1817	1820	1824	rBV	1213943	1102583	72.54%	6.956%
25	13.839	1994	1998	2001	rBV	754009	742878	48.87%	4.687%
26	15.239	2232	2236	2241	rBV	548787	706716	46.49%	4.459%

Sum of corrected areas: 15850651

LSC Report - Integrated Chromatogram

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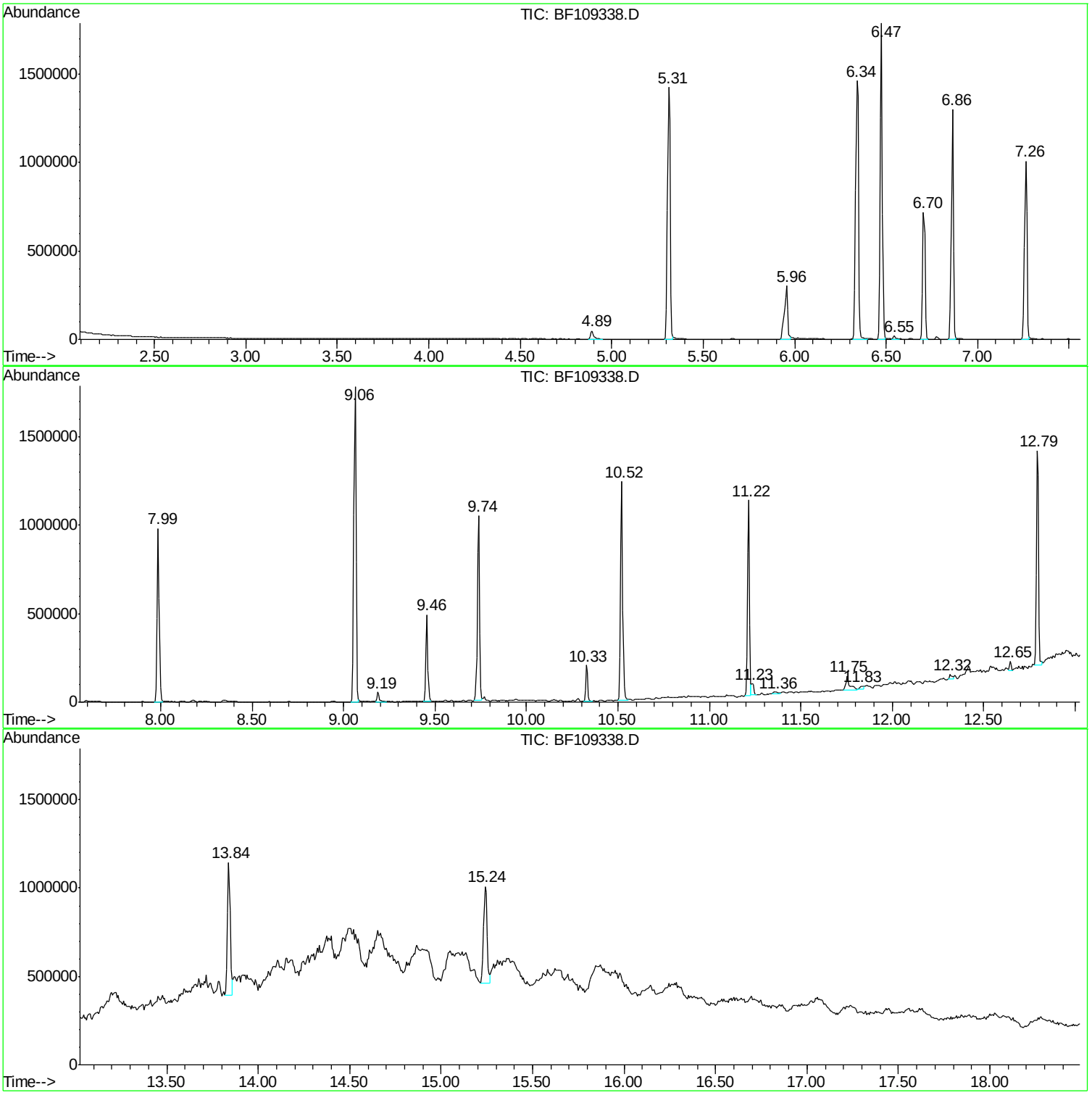
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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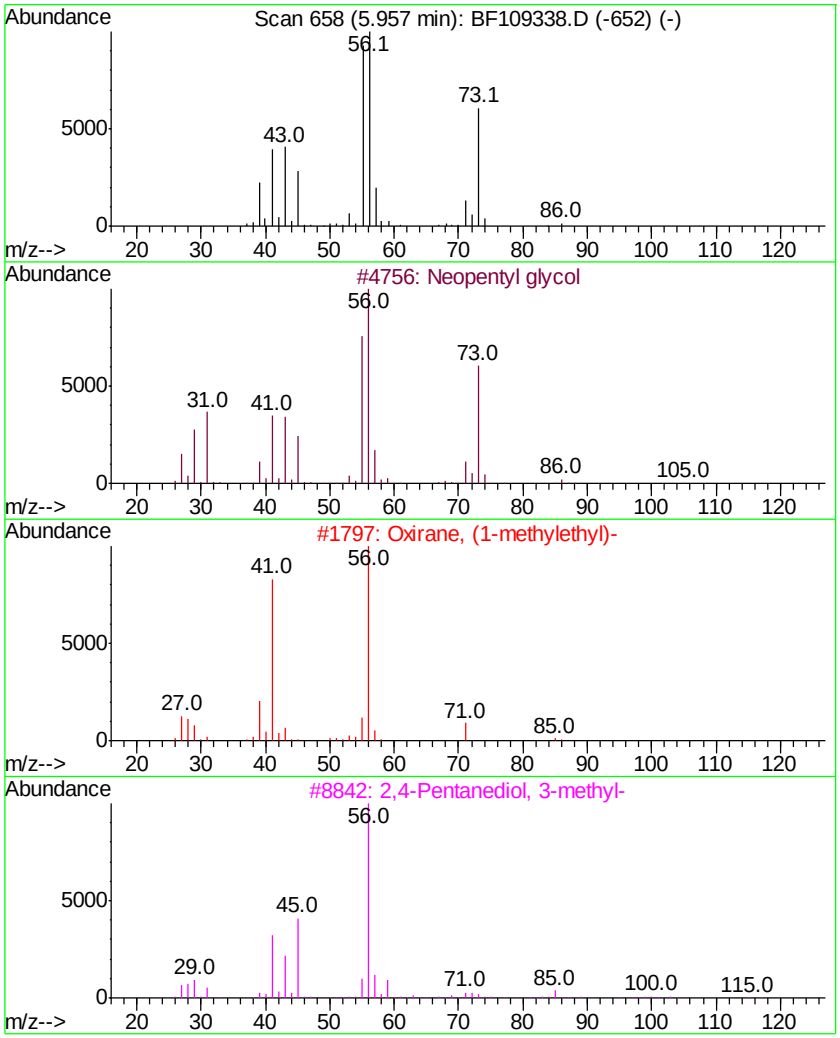
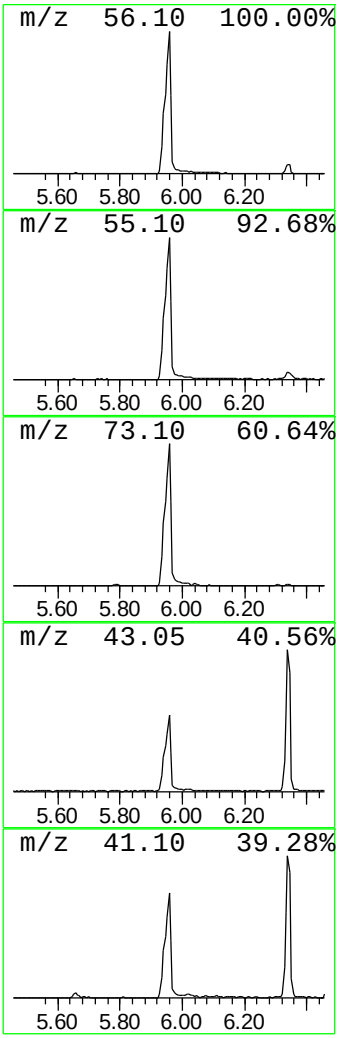
Peak Number 1 Neopentyl glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.96	12.94 ng	393366	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentyl glycol	104	C5H12O2	000126-30-7	90
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38
3	2,4-Pentanediol, 3-methyl-	118	C6H14O2	005683-44-3	36
4	Oxirane, 2-methyl-3-(1-methyleth...	100	C6H12O	001192-31-0	36
5	Pentanal, 3-methyl-	100	C6H12O	015877-57-3	33





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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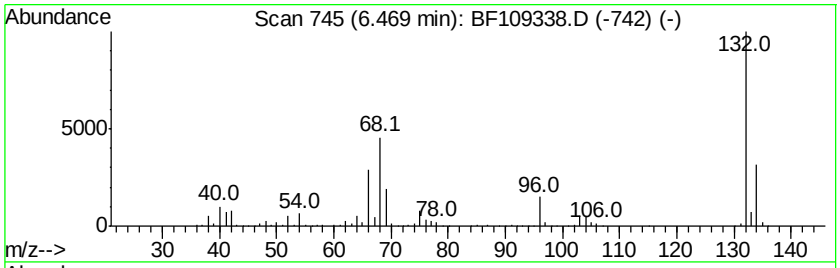
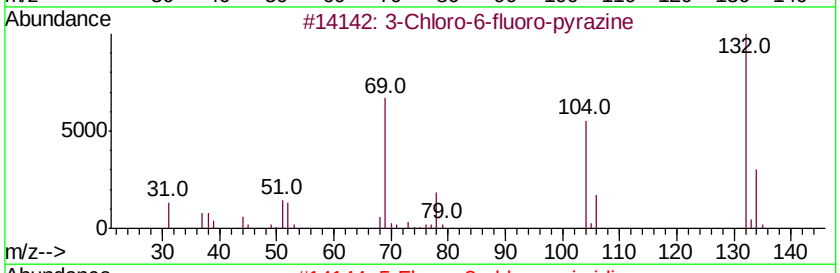
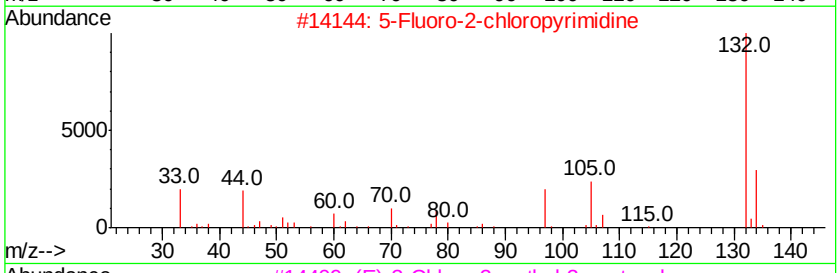
Peak Number 2 unknown6.47 Concentration Rank 1

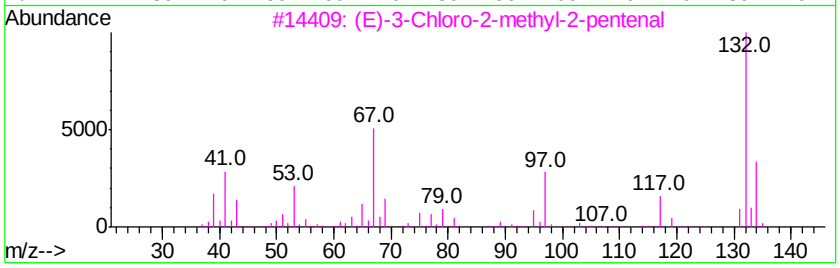
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	48.84 ng	1484960	1,4-Dichlorobenzene-d4	6.70

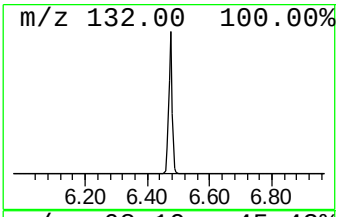
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9

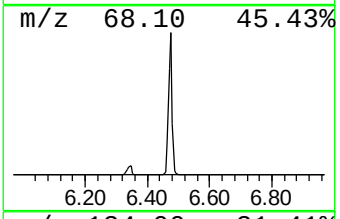


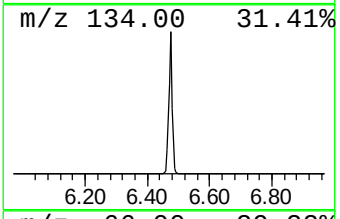


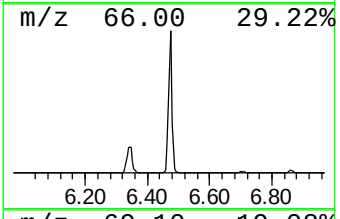


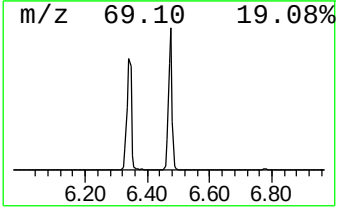












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

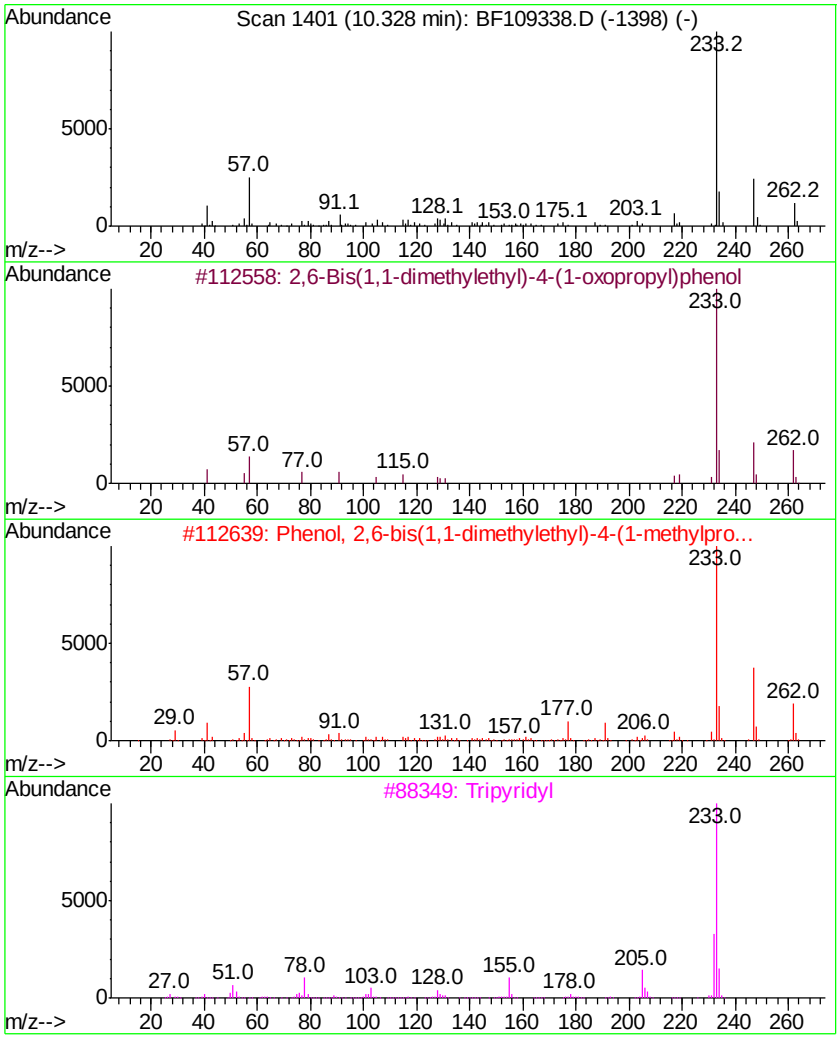
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

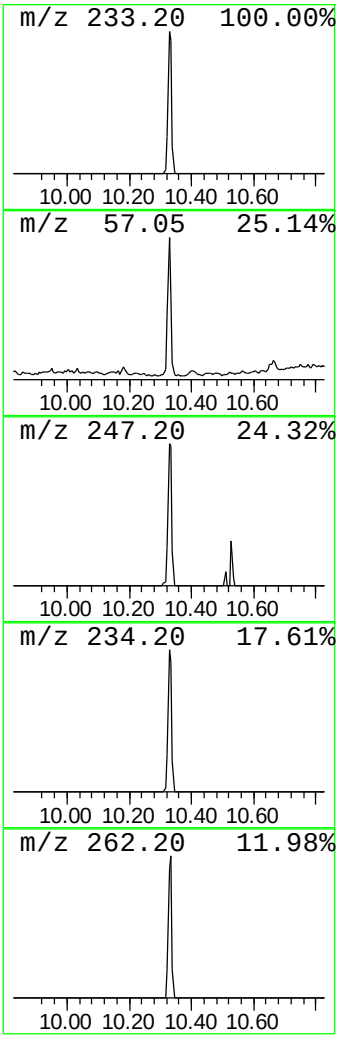
****

Peak Number 4 2,6-Bis(1,1-dimethylethyl)-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	3.55 ng	163746	Acenaphthene-d10	9.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Bis(1,1-dimethylethyl)-4-(1-...	262	C17H26O2	014035-34-8	93
2	Phenol, 2,6-bis(1,1-dimethylethy...	262	C18H30O	017540-75-9	87
3	Tripyridyl	233	C15H11N3	001148-79-4	50
4	3,5-di-tert-Butyl-4-hydroxyaceto...	248	C16H24O2	014035-33-7	50
5	Terephthalic acid, hexyl tridec-...	428	C27H40O4	1000323-92-7	47





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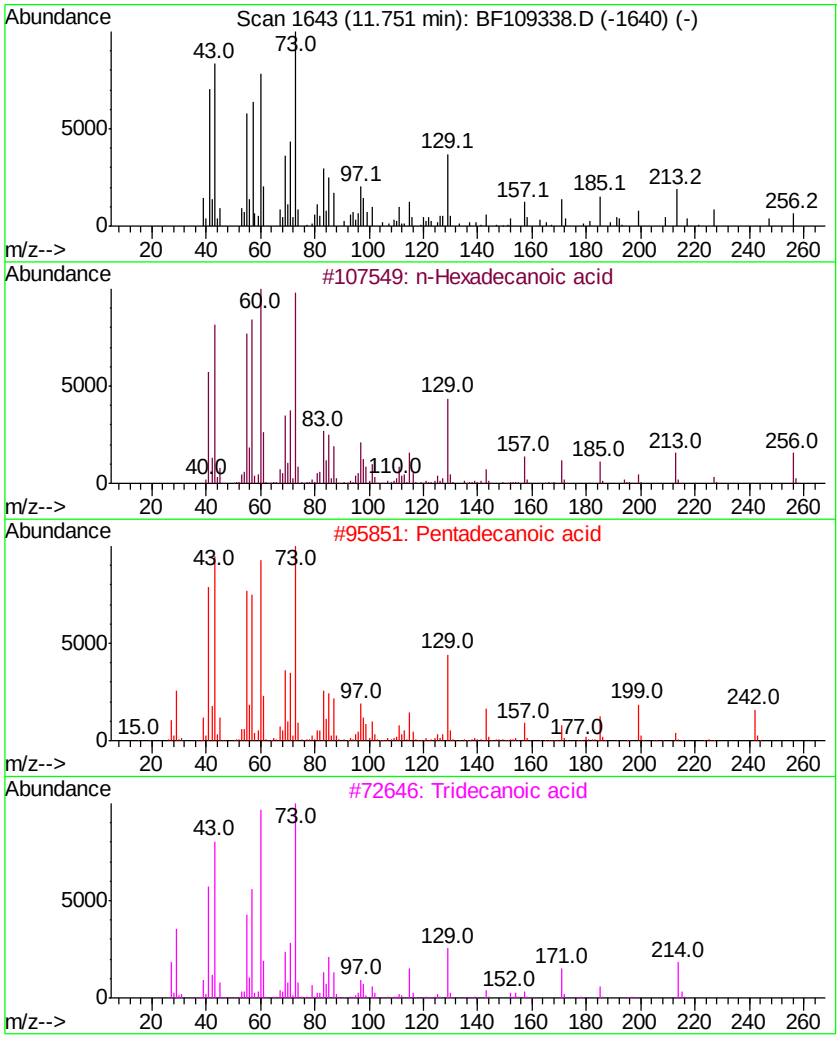
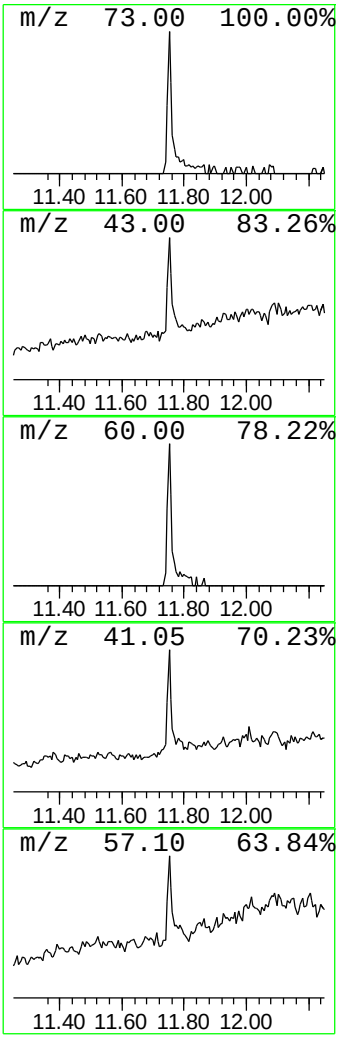
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.45 ng	112726	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	59
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Neopentyl glycol	5.96	12.9	ng	393366	1	6.70	608062	20.0
unknown6.47	6.47	48.8	ng	1484960	1	6.70	608062	20.0
2,6-Bis(1,1-dimet...	10.33	3.5	ng	163746	3	9.74	922945	20.0
n-Hexadecanoic acid	11.75	2.5	ng	112726	4	11.22	920210	20.0