LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092317\
Data File : BF098756.D
Acq On : 23 Sep 2017 23:20
Operator : SJ/JU
Sample : I5304-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-117-2(0-5)

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-BF092317.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	2.187	15	17	26	rVB2	30297	38986	1.13%	0.140%
2	2.263	26	30	45	rVB	89473	149688	4.34%	0.538%
3	5.163	518	523	535	rVB	472503	629604	18.24%	2.263%
4	5.545	583	588	591	rBV	3202846	3435513	99.50%	12.347%
5	6.545	752	758	761	rBV	3145332	3452638	100.00%	12.408%
6	6.692	778	783	786	rBV	3521875	3417699	98.99%	12.283%
7	6.922	818	822	826	rBV	1062709	853224	24.71%	3.066%
8	7.081	845	849	852	rVB	2784233	2369181	68.62%	8.515%
9	7.487	912	918	921	rBV	1928642	2005934	58.10%	7.209%
10	8.204	1036	1040	1043	rVB	1268840	1036885	30.03%	3.726%
11	9.281	1217	1223	1226	rBV	2915790	2807525	81.32%	10.090%
12	9.669	1285	1289	1292	rBV	335968	269932	7.82%	0.970%
13	9.957	1334	1338	1342	rVB	947401	892367	25.85%	3.207%
14	10.745	1467	1472	1475	rBV	1576131	1359430	39.37%	4.886%
15	10.851	1487	1490	1499	rBV	36334	41001	1.19%	0.147%
16	11.386	1578	1581	1587	rVB2	41437	39798	1.15%	0.143%
17	11.445	1587	1591	1594	rBV	986900	788582	22.84%	2.834%
18	11.822	1652	1655	1658	rBV	100252	87062	2.52%	0.313%
19	11.957	1675	1678	1683	rBV2	84034	88339	2.56%	0.317%
20	12.239	1724	1726	1729	rBV	52213	44805	1.30%	0.161%
21	12.839	1826	1828	1831	rVB	45985	42017	1.22%	0.151%
22	13.027	1856	1860	1864	rBV	2380538	2213112	64.10%	7.954%
23	13.916	2008	2011	2014	rBV	104742	111870	3.24%	0.402%
24	14.086	2036	2040	2043	rBV	881946	793666	22.99%	2.852%
25	14.804	2160	2162	2167	rVB	95594	105058	3.04%	0.378%
26	15.580	2289	2294	2303	rVB	516968	750944	21.75%	2.699%

Sum of corrected areas: 27824860

LSC Report - Integrated Chromatogram

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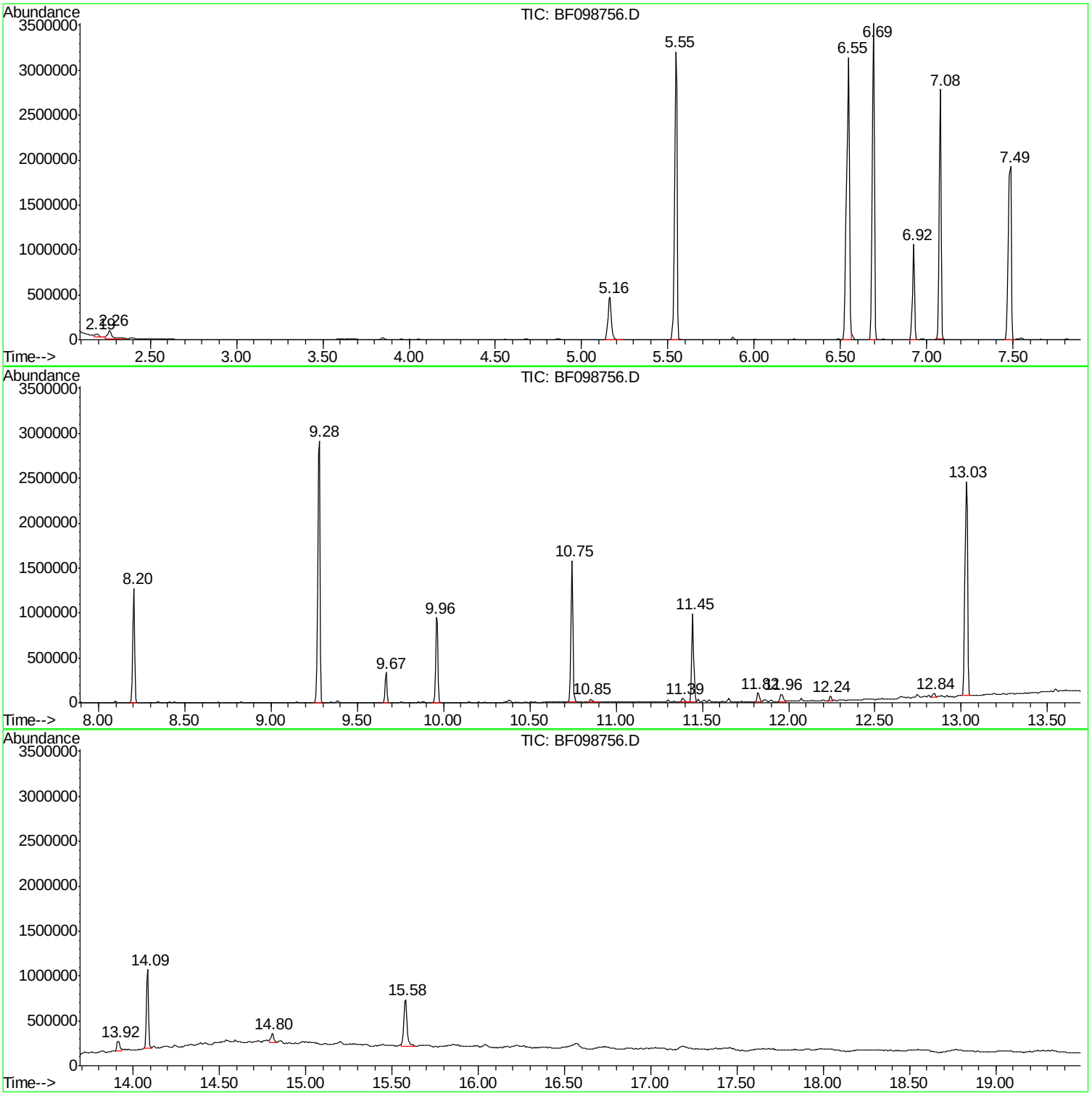
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-117-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF092317\
Data File : BF098756.D
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Sample : I5304-01
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Instrument : BNA_F
ClientSampleId : SASP2P-ENV-117-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

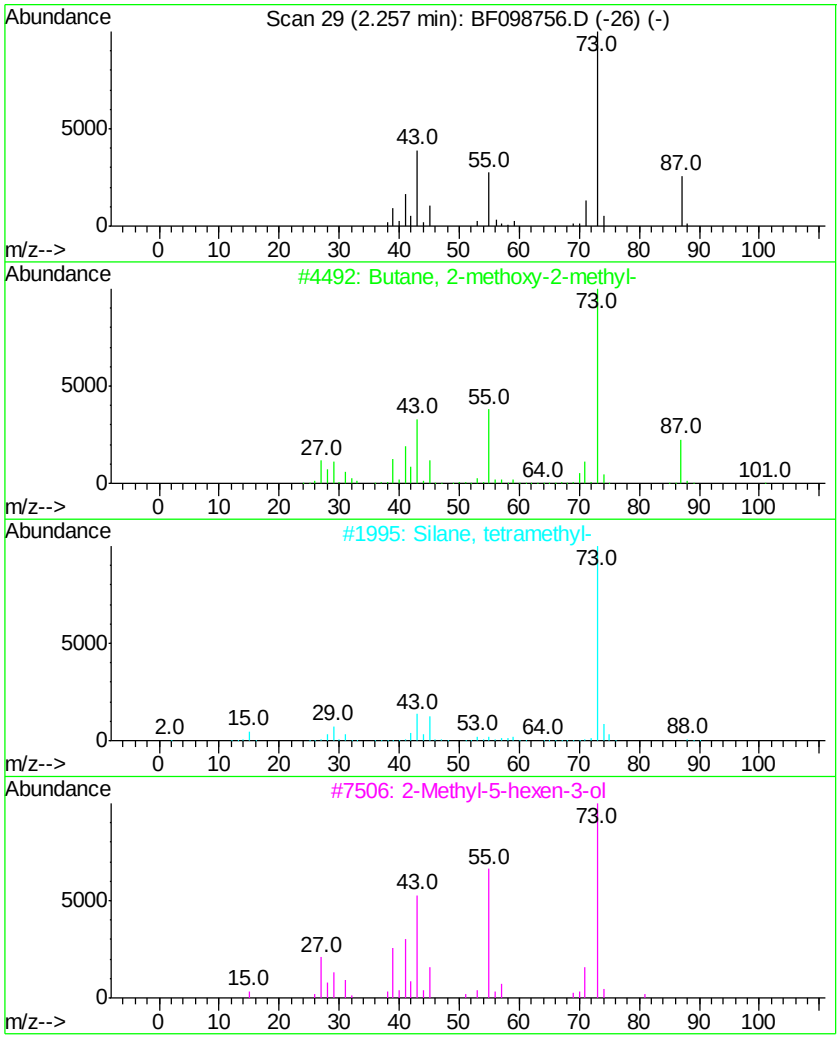
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

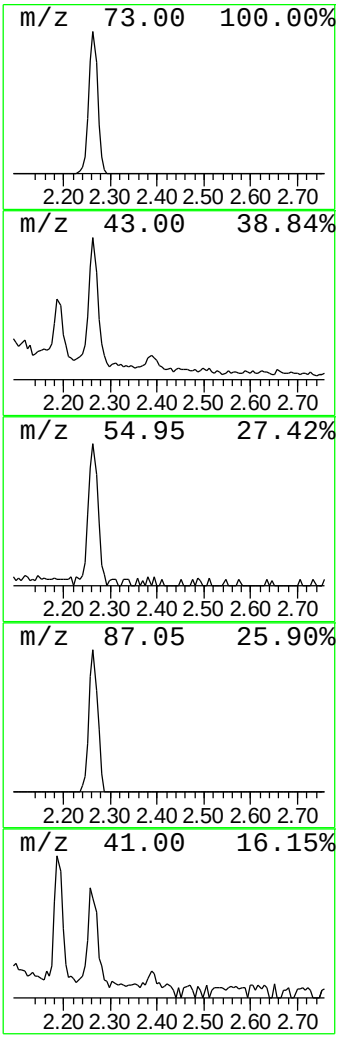
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	3.51 ng	149688	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	27
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10





Library Search Compound Report

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Data File : BF098756.D
Acq On : 23 Sep 2017 23:20
Operator : SJ/JU
Sample : I5304-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-117-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

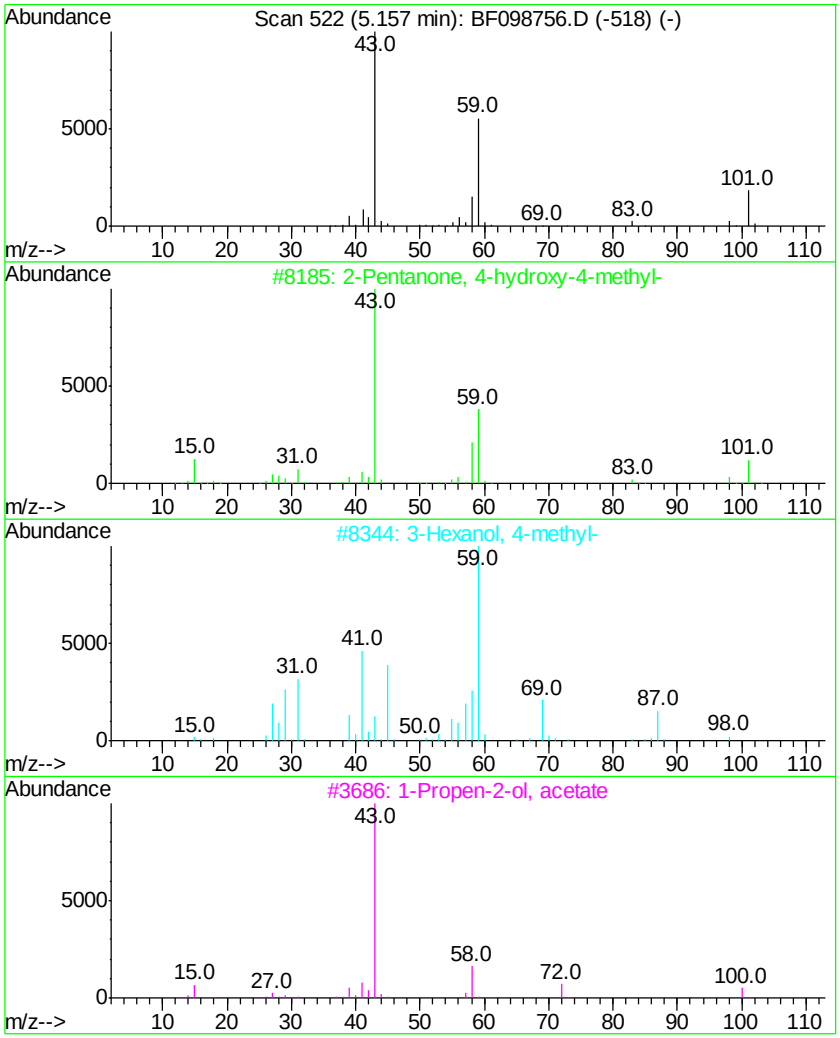
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

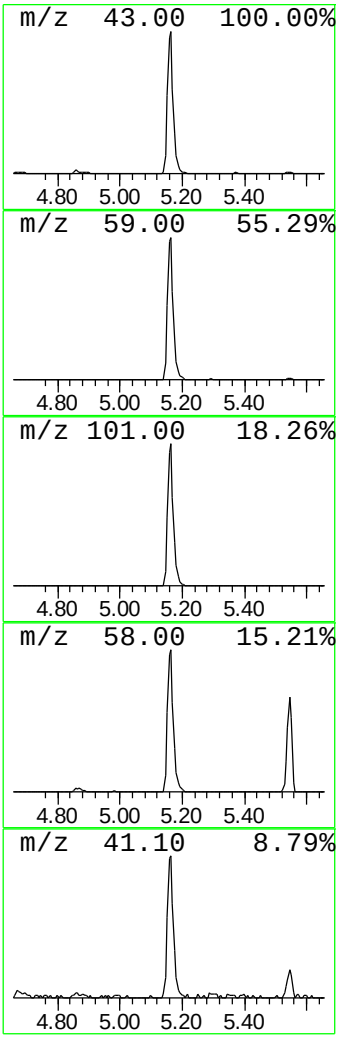
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	14.76 ng	629604	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092317\
Data File : BF098756.D
Acq On : 23 Sep 2017 23:20
Operator : SJ/JU
Sample : I5304-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-117-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

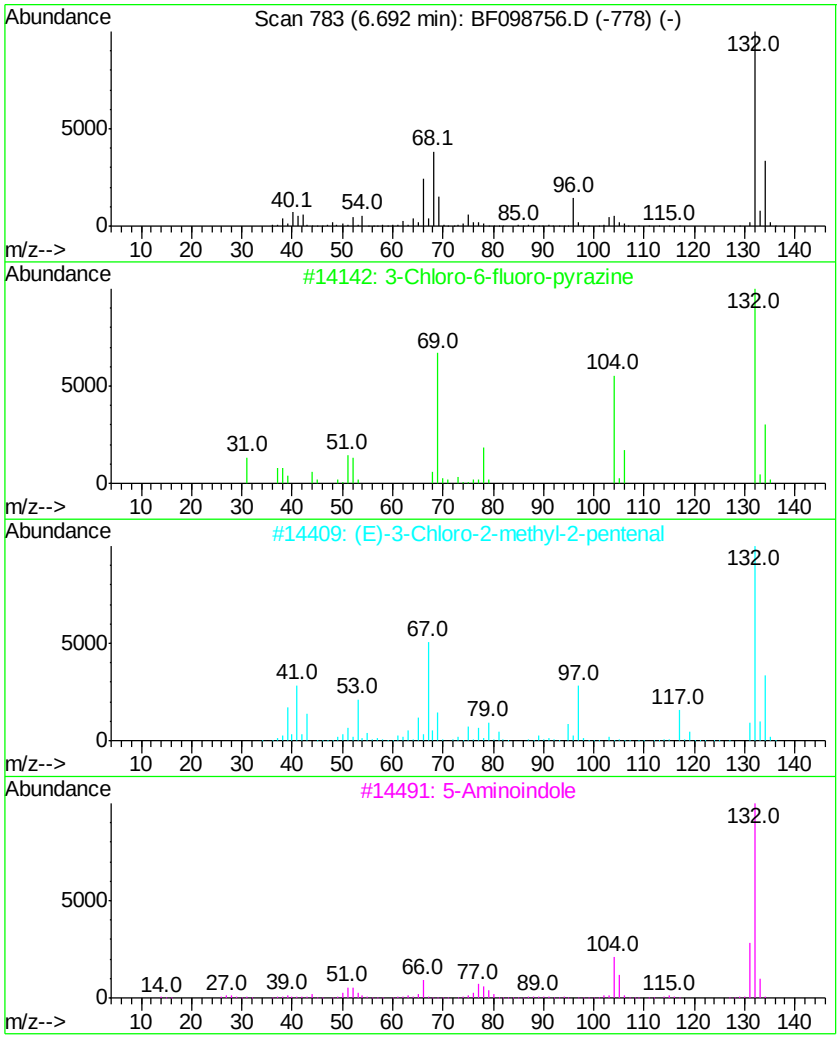
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

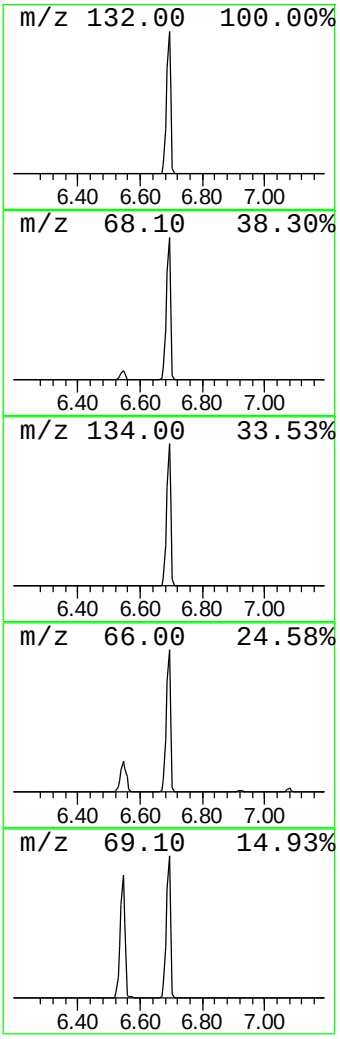
****

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	80.11 ng	3417700	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Operator : SJ/JU
Sample : I5304-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-117-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

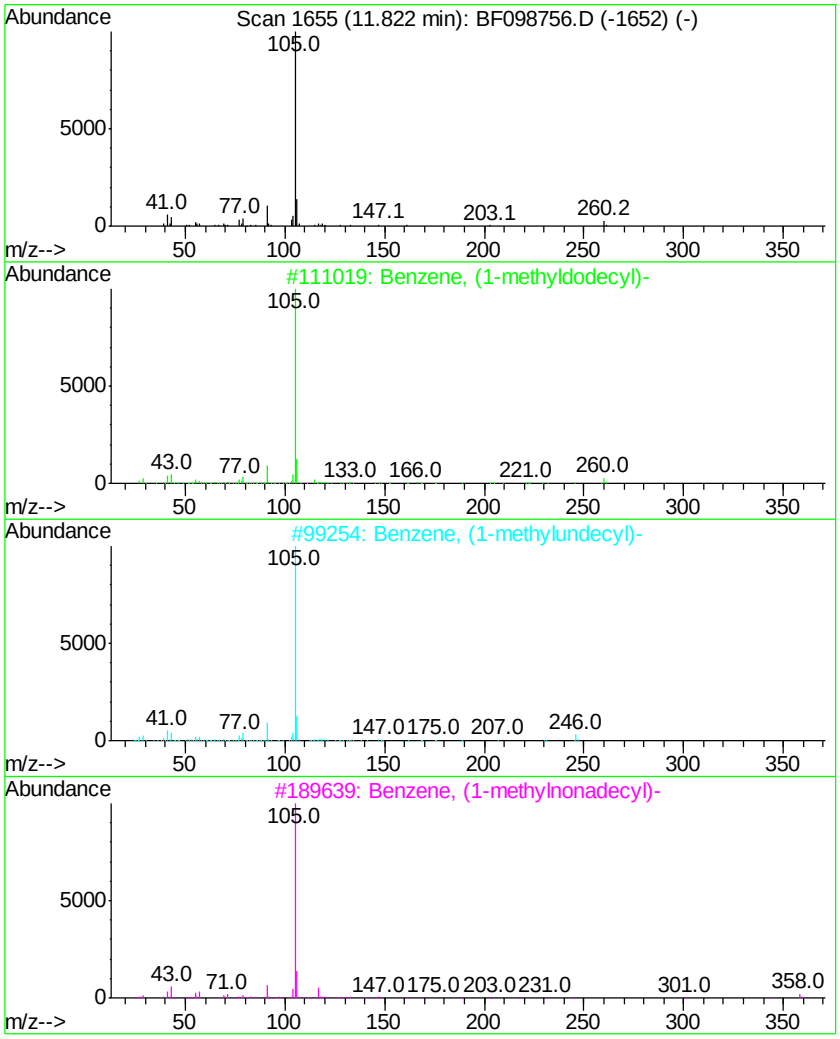
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

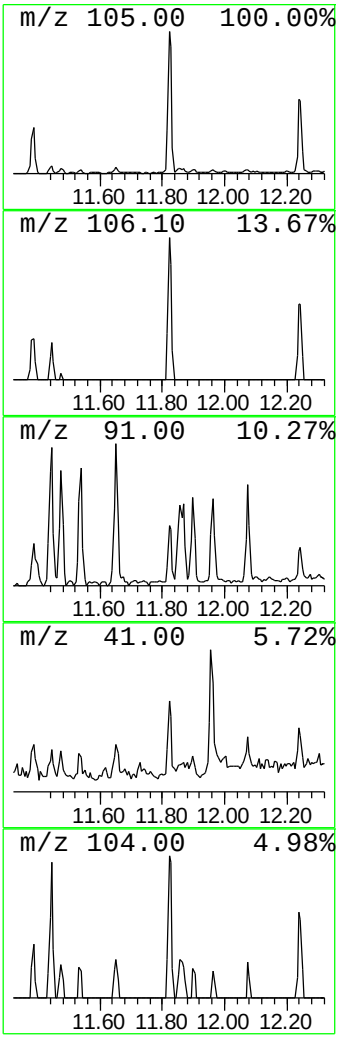
****

Peak Number 5 Benzene, (1-methyldodecyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.21 ng	87062	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	81
2	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	72
3	Benzene, (1-methylnonadecyl)-	358	C26H46	002398-66-5	59
4	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	56
5	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	50





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Operator : SJ/JU
Sample : I5304-01
Misc :
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Instrument : BNA_F
ClientSampleId : SASP2P-ENV-117-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

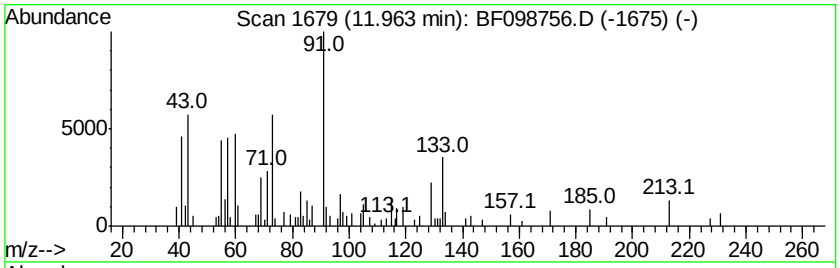
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

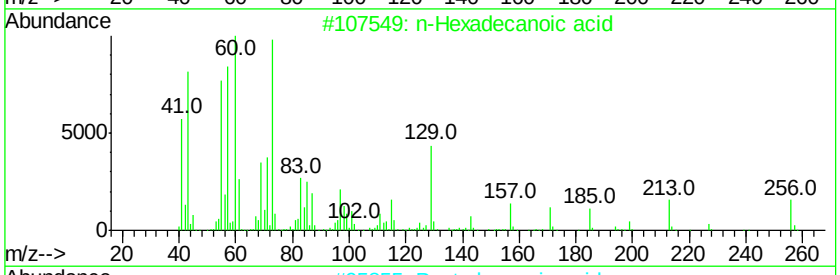
****

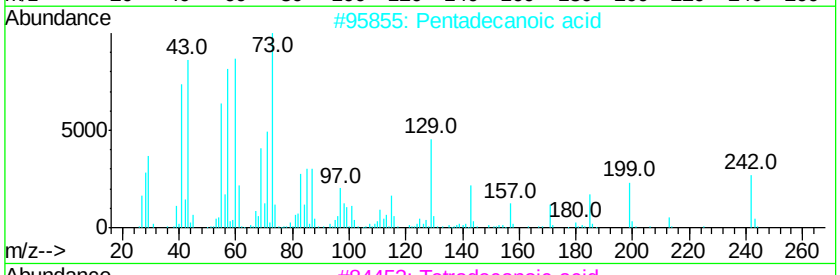
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

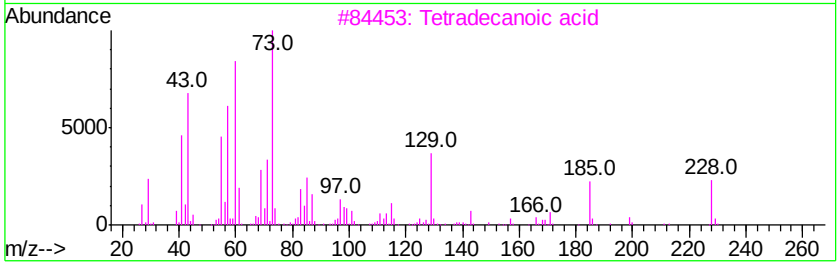
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	2.24 ng	88339	Phenanthrene-d10	11.45

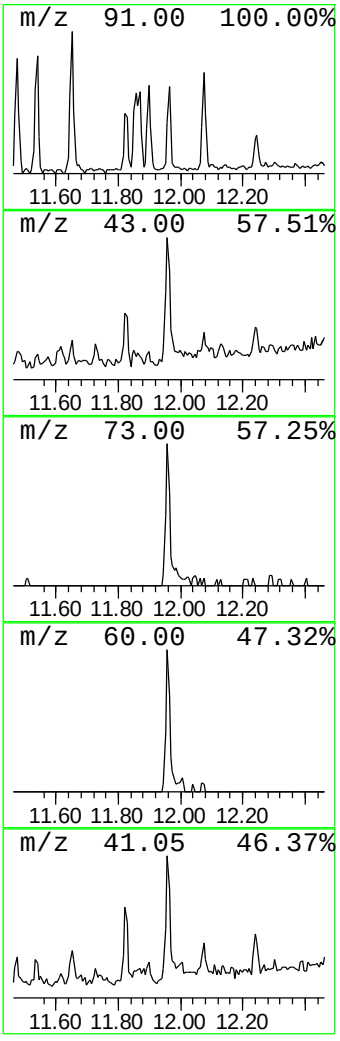
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72











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SASP2P-ENV-117-2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

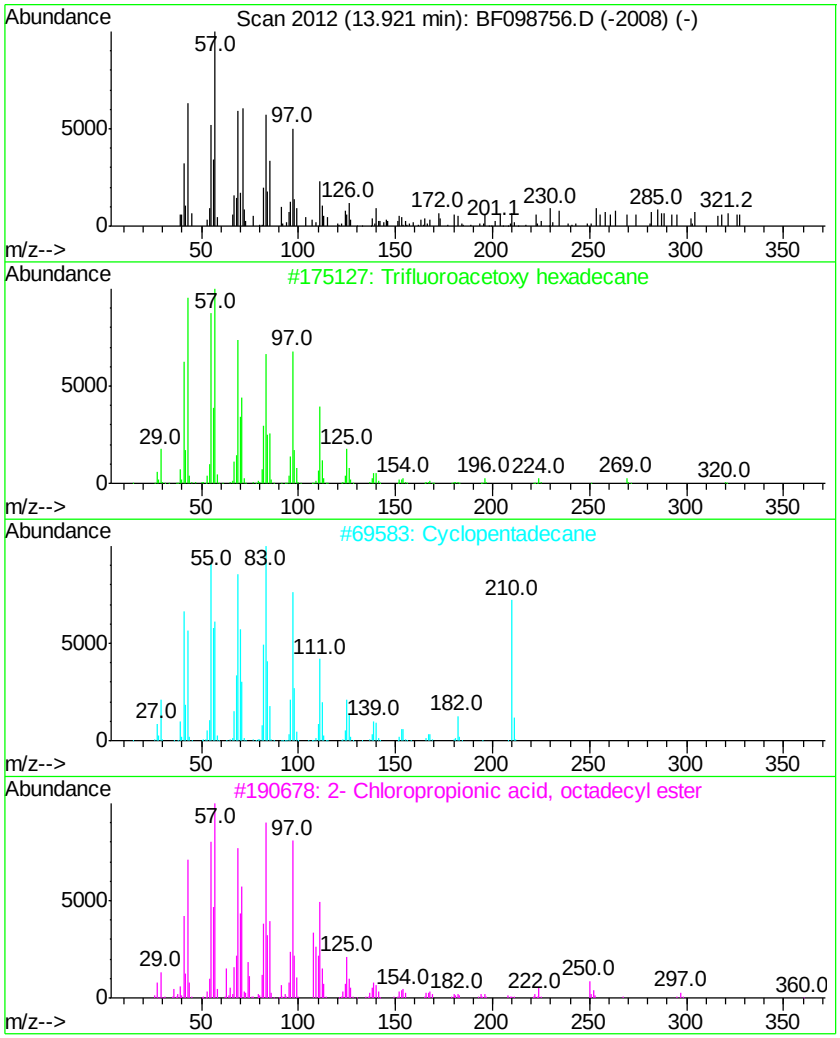
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

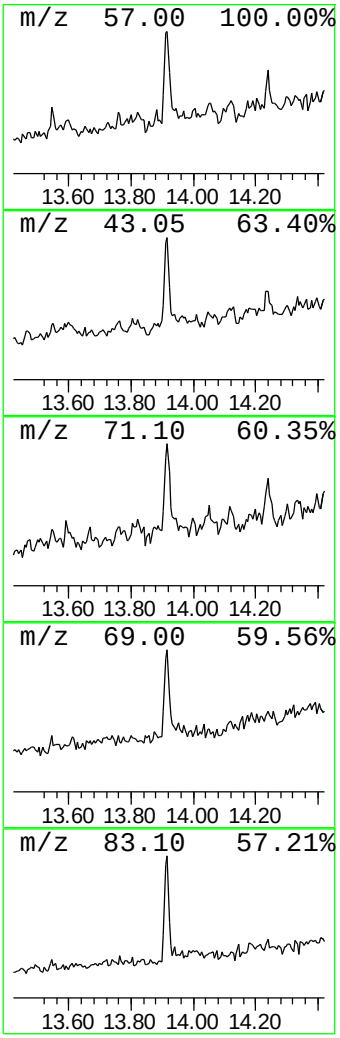
****

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	2.82 ng	111870	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Cyclopentadecane	210	C15H30	000295-48-7	95
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94





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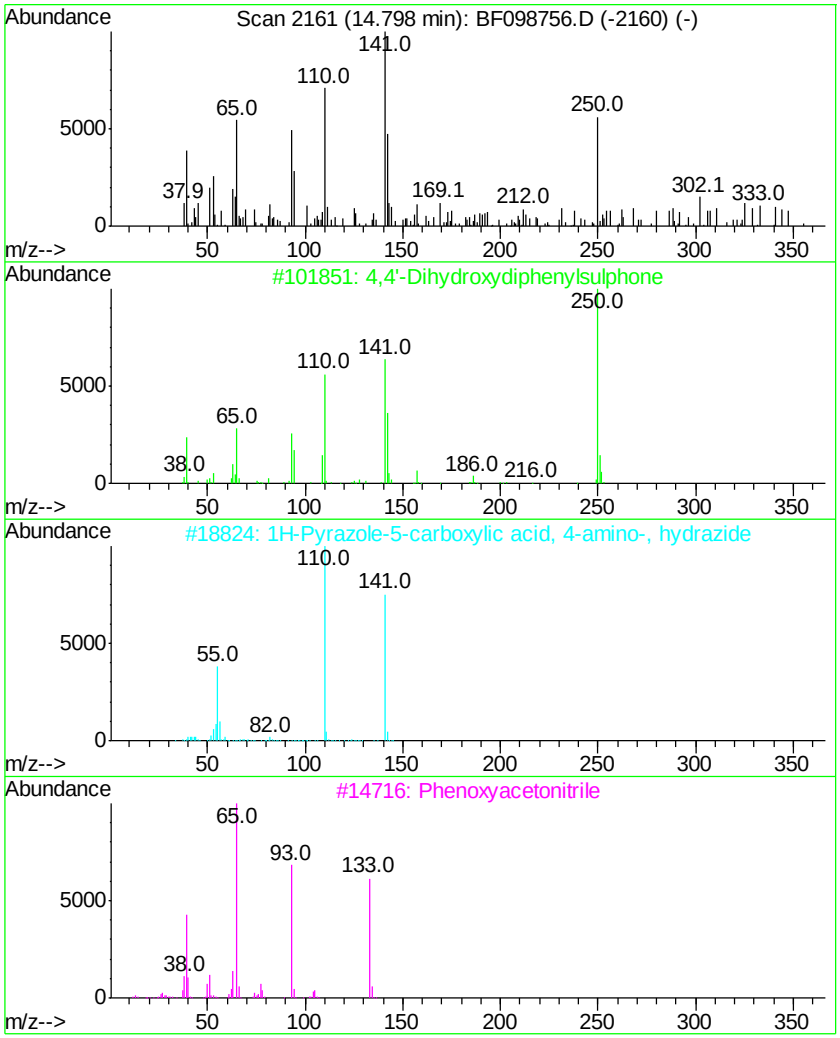
TIC Integration Parameters: LSCINT.P

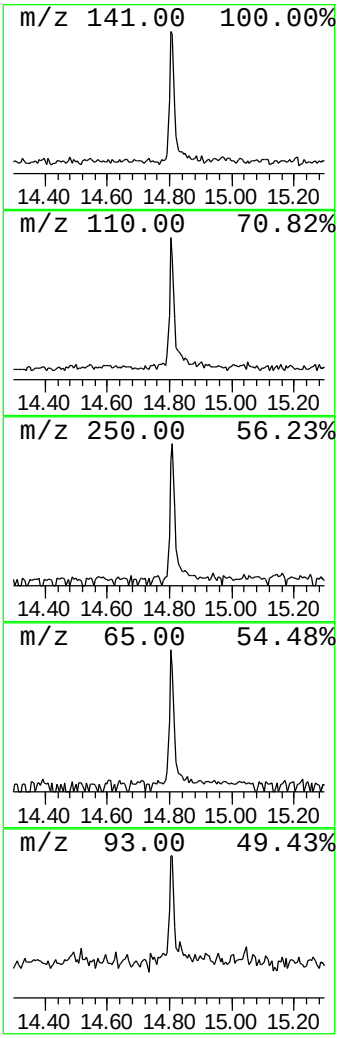
****

Peak Number 8 4,4'-Dihydroxydiphenylsulphone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	2.65 ng	105058	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	96
2	1H-Pyrazole-5-carboxylic acid, 4...	141	C4H7N5O	1000327-48-2	14
3	Phenoxyacetonitrile	133	C8H7NO	003598-14-9	12
4	Naphthalene, 2-butyl-	184	C14H16	001134-62-9	10
5	Naphthalene, 1-hexyl-	212	C16H20	002876-53-1	10





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
Butane, 2-methoxy...	2.26	3.5	ng	149688	1	6.92	853224	20.0
2-Pentanone, 4-hy...	5.16	14.8	ng	629604	1	6.92	853224	20.0
unknown6.69	6.69	80.1	ng	3417700	1	6.92	853224	20.0
Benzene, (1-methy...	11.82	2.2	ng	87062	4	11.45	788582	20.0
n-Hexadecanoic acid	11.96	2.2	ng	88339	4	11.45	788582	20.0
Trifluoroacetoxy ...	13.92	2.8	ng	111870	5	14.09	793666	20.0
4,4'-Dihydroxydip...	14.80	2.6	ng	105058	5	14.09	793666	20.0