LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104495.D
Acq On : 13 Apr 2018 22:42
Operator : JU/SJ
Sample : PB108218BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB108218BL

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-BF040618.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	5.016	494	498	506	rVB	78949	88046	4.41%	0.509%
2	5.434	564	569	572	rBV	1729195	1740141	87.08%	10.069%
3	5.751	619	623	627	rVB	56338	49848	2.49%	0.288%
4	6.445	737	741	744	rBV	1696149	1684148	84.28%	9.745%
5	6.581	760	764	767	rBV	2141366	1788305	89.49%	10.348%
6	6.810	799	803	806	rBV	975699	737514	36.91%	4.268%
7	6.963	825	829	833	rBV	1634890	1459265	73.02%	8.444%
8	7.375	894	899	902	rBV	1232833	1067932	53.44%	6.180%
9	8.092	1017	1021	1024	rBV	1196083	914074	45.74%	5.289%
10	9.169	1200	1204	1207	rBV	2427550	1998357	100.00%	11.563%
11	9.563	1267	1271	1274	rBV	111322	93191	4.66%	0.539%
12	9.774	1303	1307	1310	rBV	63154	46746	2.34%	0.270%
13	9.851	1316	1320	1329	rVB	1030613	924943	46.29%	5.352%
14	10.245	1384	1387	1390	rBV2	24925	23921	1.20%	0.138%
15	10.274	1390	1392	1395	rVB	82371	57761	2.89%	0.334%
16	10.639	1450	1454	1465	rVB	983623	846748	42.37%	4.900%
17	10.751	1470	1473	1478	rBV	58497	59185	2.96%	0.342%
18	11.339	1569	1573	1576	rBV	905927	749075	37.48%	4.334%
19	12.927	1839	1843	1846	rBV	1599095	1408119	70.46%	8.148%
20	13.815	1991	1994	1997	rBV	178108	171754	8.59%	0.994%
21	13.851	1997	2000	2005	rVB	137684	114445	5.73%	0.662%
22	13.980	2018	2022	2026	rBV	725320	648847	32.47%	3.755%
23	14.833	2163	2167	2170	rVB	38444	40890	2.05%	0.237%
24	15.451	2266	2272	2280	rBV	385186	514048	25.72%	2.974%
25	15.898	2345	2348	2353	rVB3	16959	23573	1.18%	0.136%
26	15.951	2354	2357	2364	rVB6	16156	30956	1.55%	0.179%

Sum of corrected areas: 17281832

LSC Report - Integrated Chromatogram

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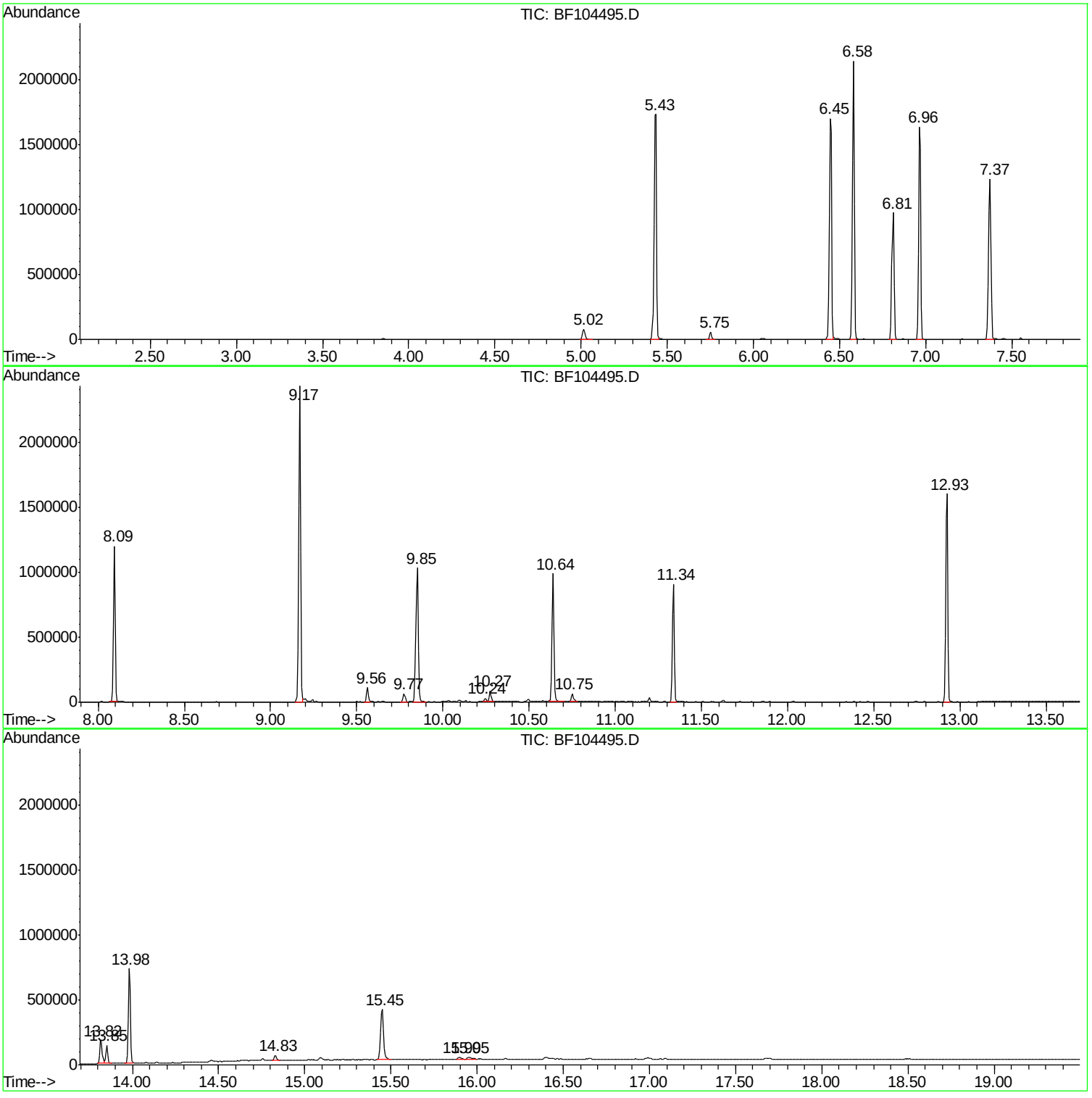
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB108218BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104495.D
Acq On : 13 Apr 2018 22:42
Operator : JU/SJ
Sample : PB108218BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB108218BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

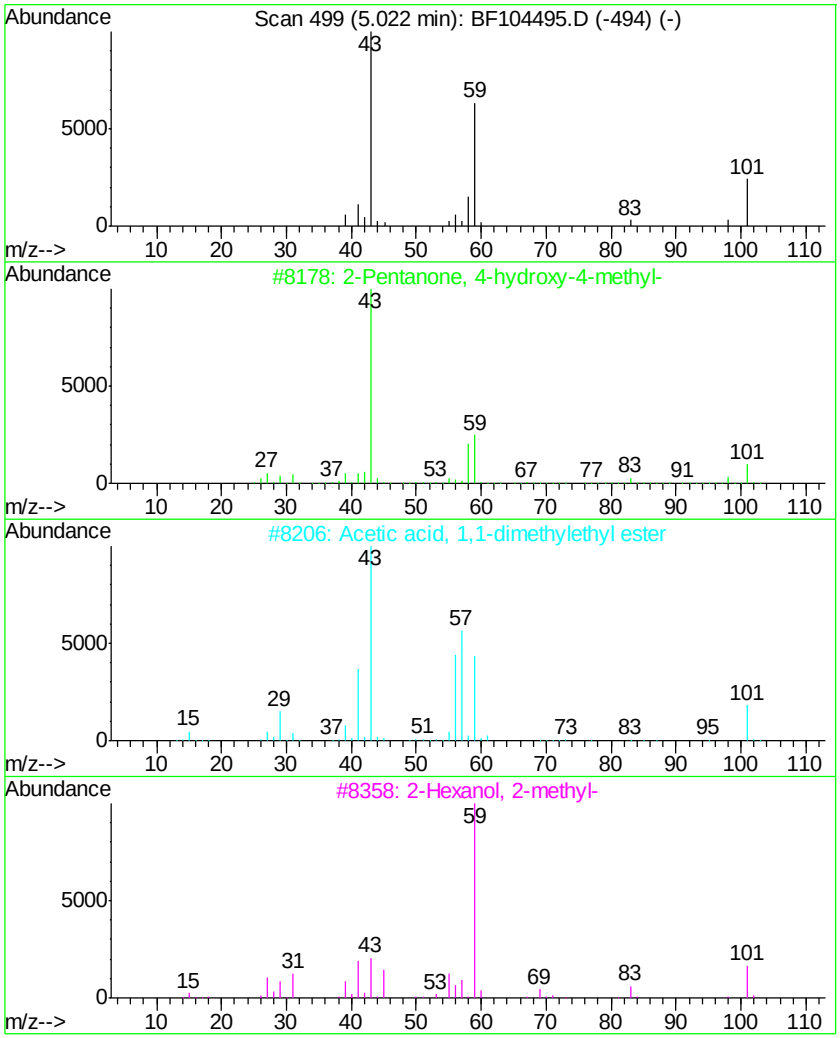
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

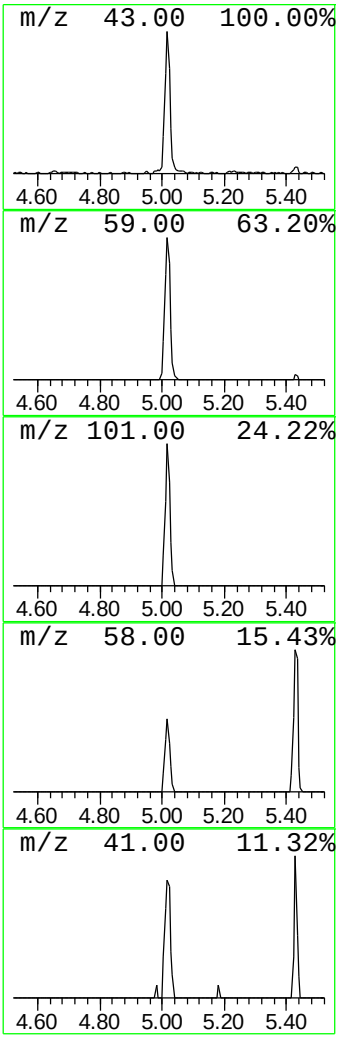
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	2.39 ng	88046	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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Data File : BF104495.D
Acq On : 13 Apr 2018 22:42
Operator : JU/SJ
Sample : PB108218BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB108218BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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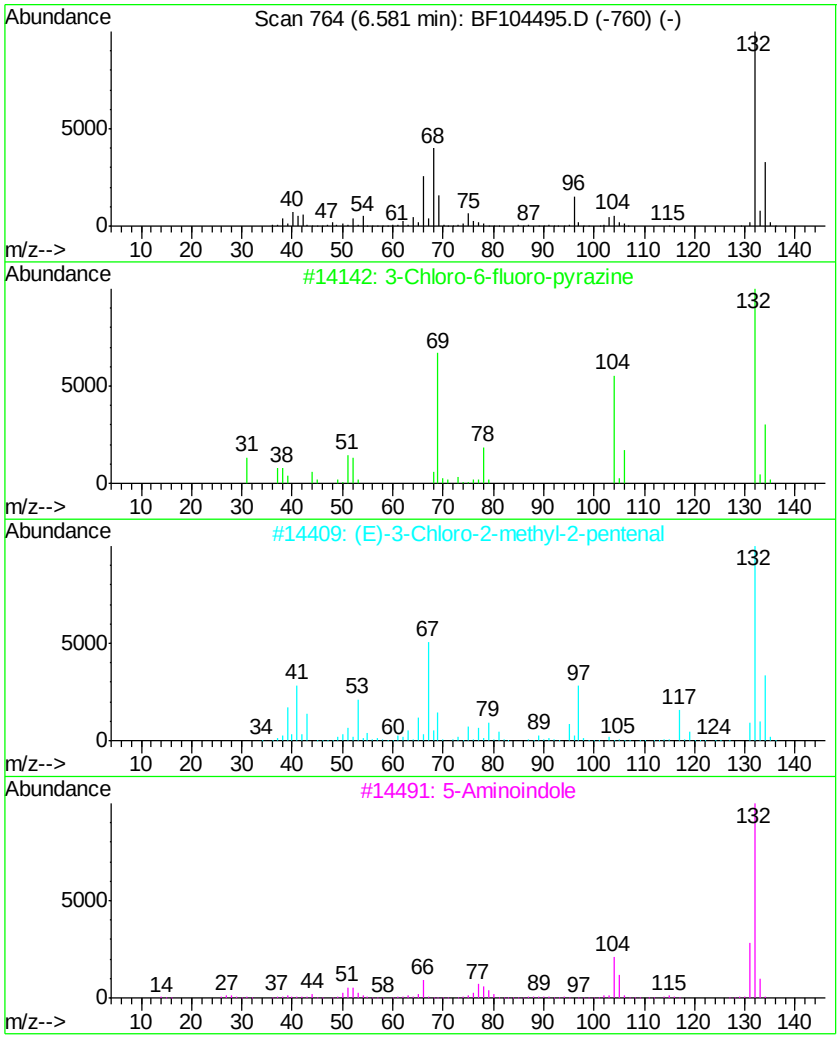
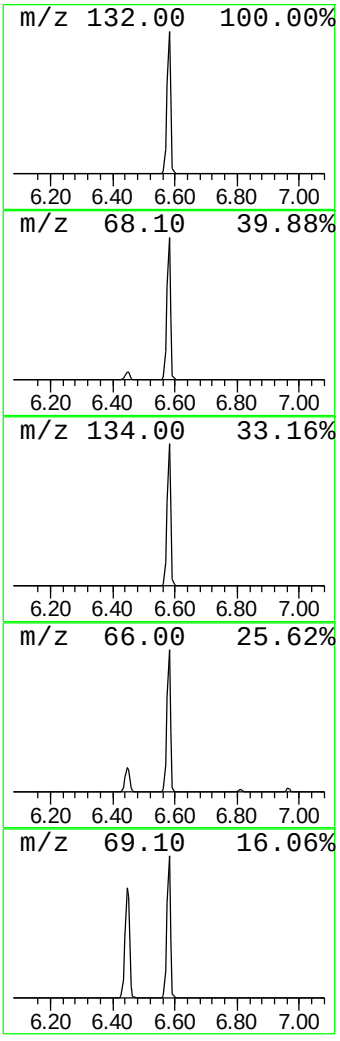
Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	48.50 ng	1788310	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Operator : JU/SJ
Sample : PB108218BL
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB108218BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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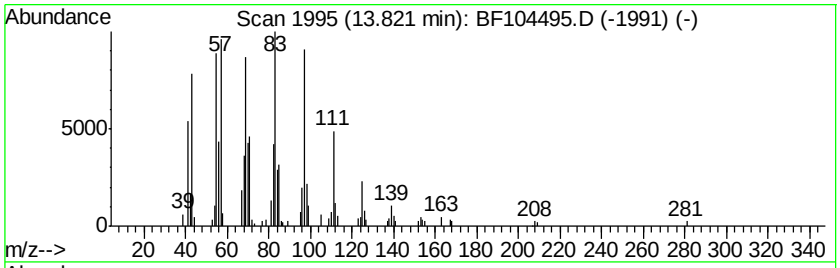
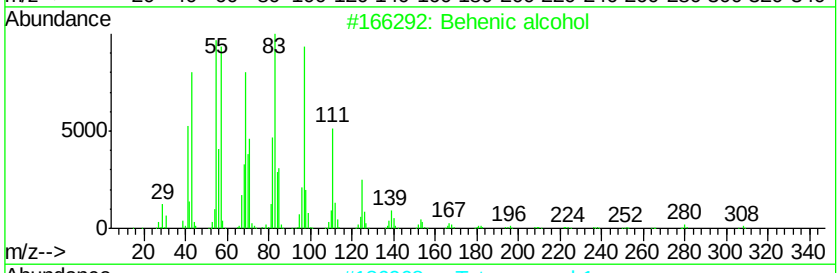
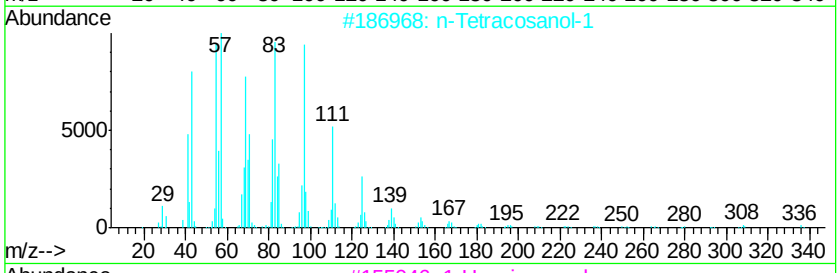
Peak Number 4 Behenic alcohol Concentration Rank 3

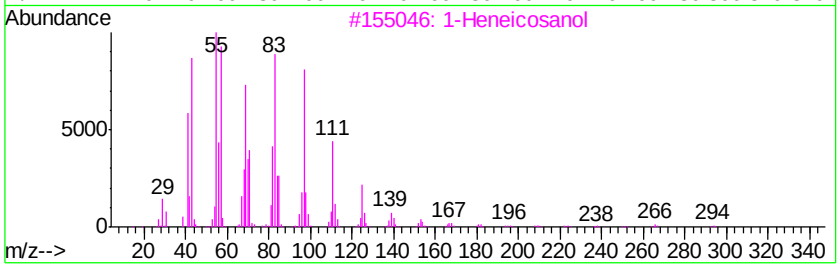
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	5.29 ng	171754	Chrysene-d12	13.98

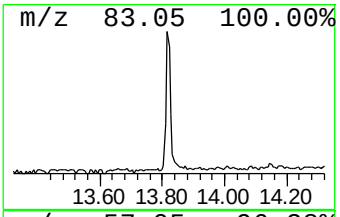
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93

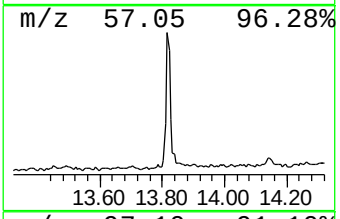


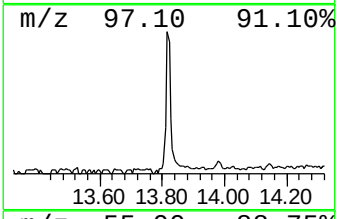


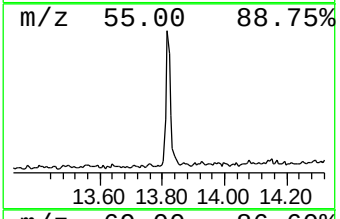


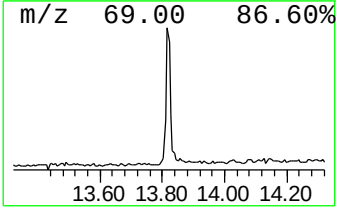












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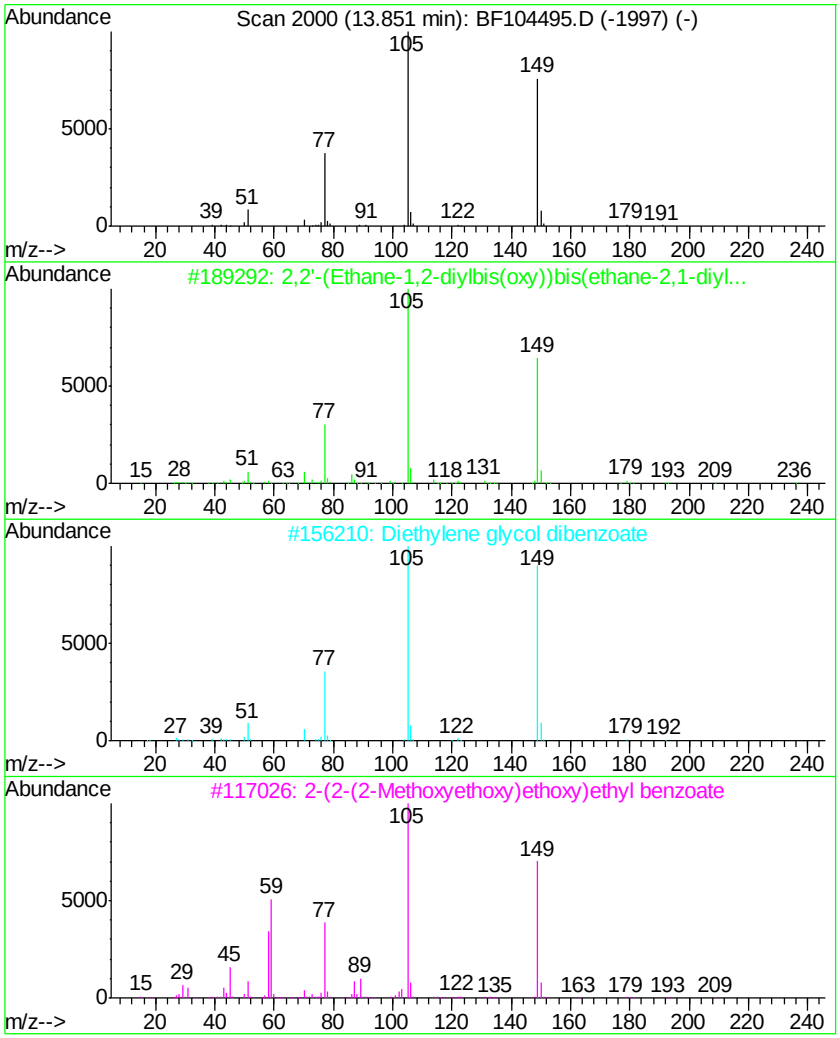
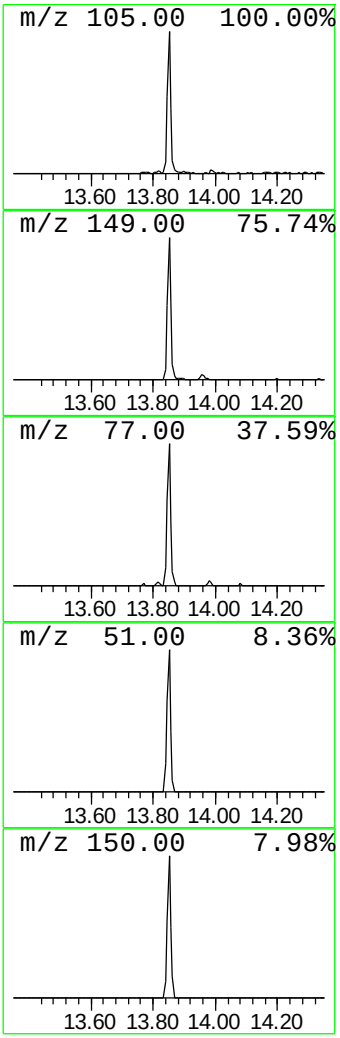
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.53 ng	114445	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
3	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
4	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	74
5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64





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...	5.02	2.4	ng	88046	1	6.81	737514	20.0
unknown6.58	6.58	48.5	ng	1788310	1	6.81	737514	20.0
Behenic alcohol	13.82	5.3	ng	171754	5	13.98	648847	20.0
2,2'-(Ethane-1,2-...	13.85	3.5	ng	114445	5	13.98	648847	20.0