LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022317\
Data File : BF093117.D
Acq On : 23 Feb 2017 21:13
Operator : SJ/MA
Sample : I1954-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CLP-S-04(5-10)

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-BF013017.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	5.013	253	256	266	rBV	1016965	1672381	40.54%	4.437%
2	5.436	290	293	295	rBV	3809010	3829956	92.83%	10.162%
3	6.476	381	384	387	rBV	3183565	3787652	91.81%	10.050%
4	6.601	393	395	398	rBV	3035485	3854747	93.44%	10.228%
5	6.841	413	416	418	rBV	677237	916784	22.22%	2.433%
6	6.990	427	429	432	rBV	2916185	2835894	68.74%	7.525%
7	7.402	462	465	468	rBV	2104450	2392768	58.00%	6.349%
8	8.122	526	528	530	rBV	1507552	1321582	32.03%	3.507%
9	9.196	619	622	625	rBV	3554049	4125574	100.00%	10.946%
10	9.596	654	657	659	rBV	364576	334293	8.10%	0.887%
11	9.802	672	675	679	rBV	48017	70089	1.70%	0.186%
12	9.870	679	681	684	rVB	1399021	1422785	34.49%	3.775%
13	10.282	715	717	718	rBV	33261	50221	1.22%	0.133%
14	10.305	718	719	721	rVB	134657	95864	2.32%	0.254%
15	10.522	735	738	741	rBV	44481	63384	1.54%	0.168%
16	10.659	748	750	753	rBV2	1862870	2285695	55.40%	6.065%
17	10.773	758	760	767	rVB	178451	212942	5.16%	0.565%
18	11.219	797	799	801	rBV	118671	123203	2.99%	0.327%
19	11.356	809	811	813	rBV	1694660	1464954	35.51%	3.887%
20	11.653	834	837	839	rBV	66499	88489	2.14%	0.235%
21	12.945	947	950	952	rBV	3959877	3974968	96.35%	10.547%
22	13.836	1026	1028	1038	rBV	146036	233054	5.65%	0.618%
23	13.996	1039	1042	1044	rBV	1111081	1355557	32.86%	3.597%
24	14.819	1112	1114	1117	rVB	104878	133520	3.24%	0.354%
25	15.414	1164	1166	1173	rVB	777673	1042422	25.27%	2.766%

Sum of corrected areas: 37688778

LSC Report - Integrated Chromatogram

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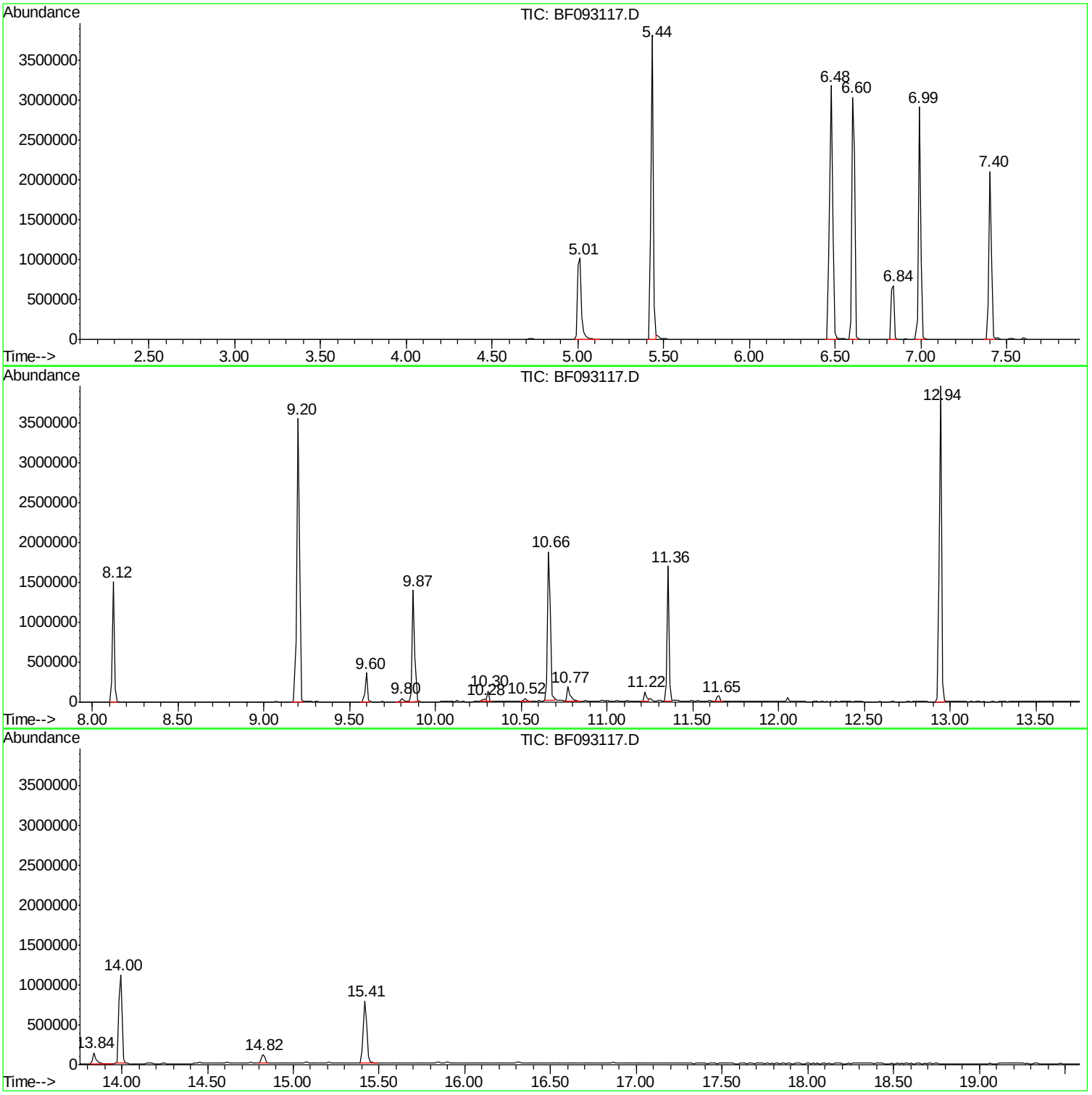
Instrument : BNA_F
ClientSampleId : CLP-S-04(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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TIC Integration Parameters: LSCINT.P

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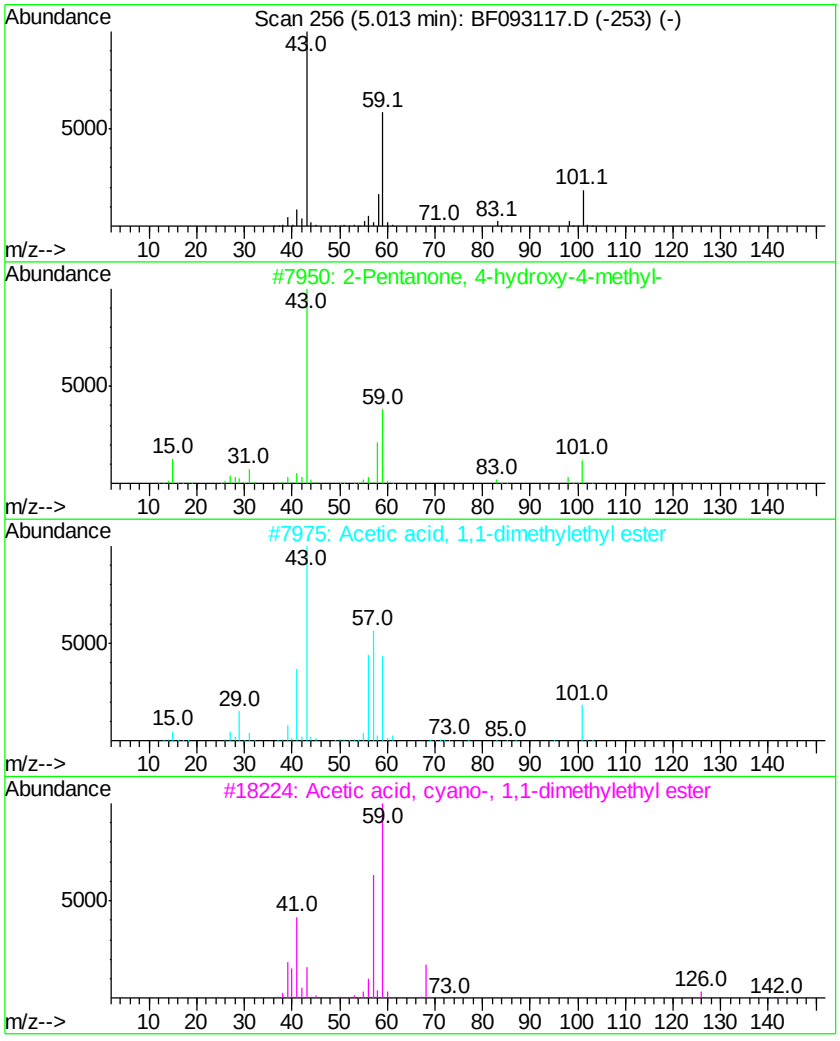
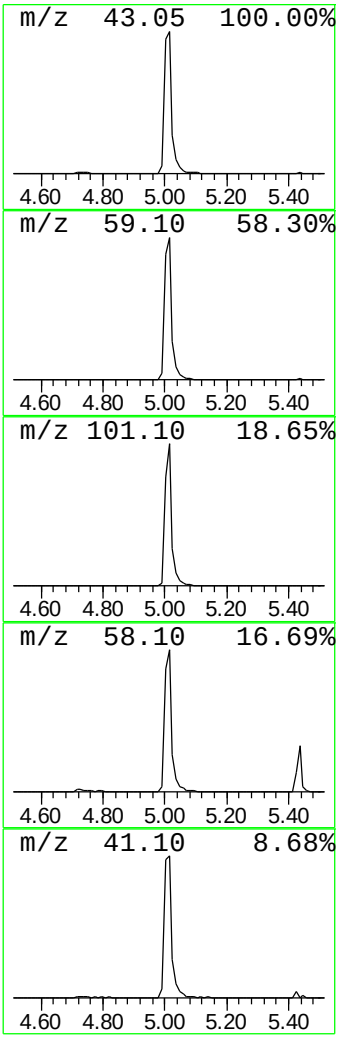
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	36.48 ng	1672380	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CLP-S-04(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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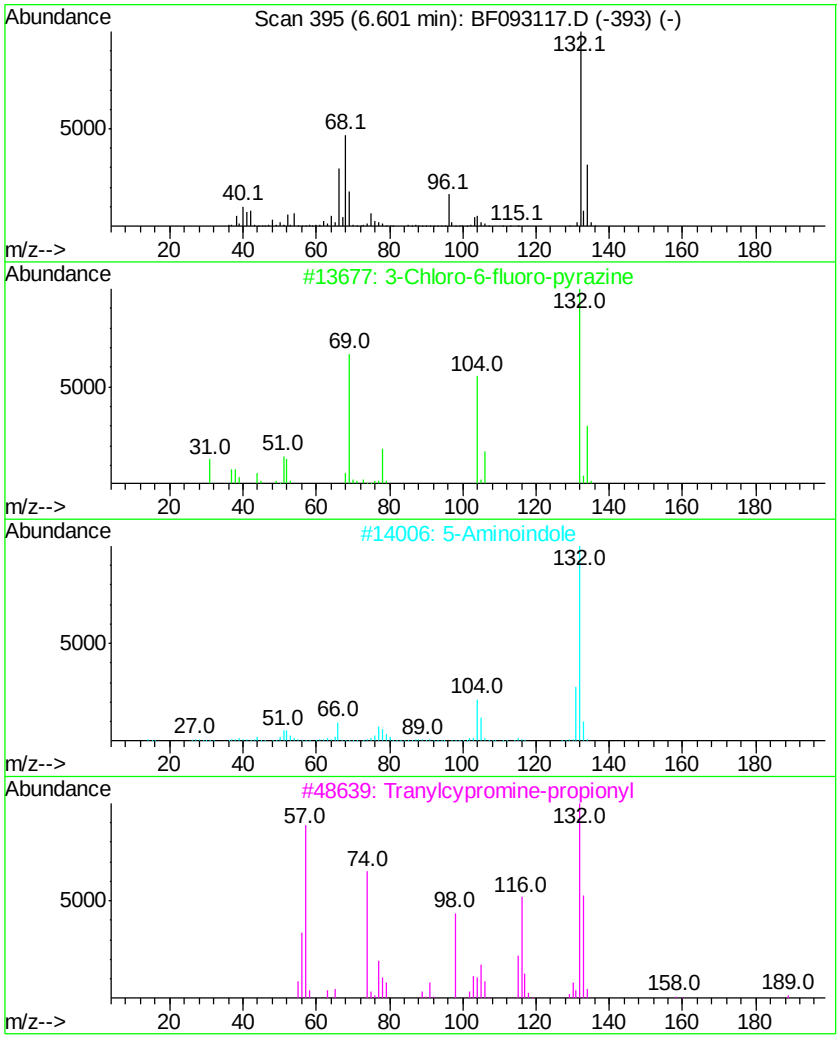
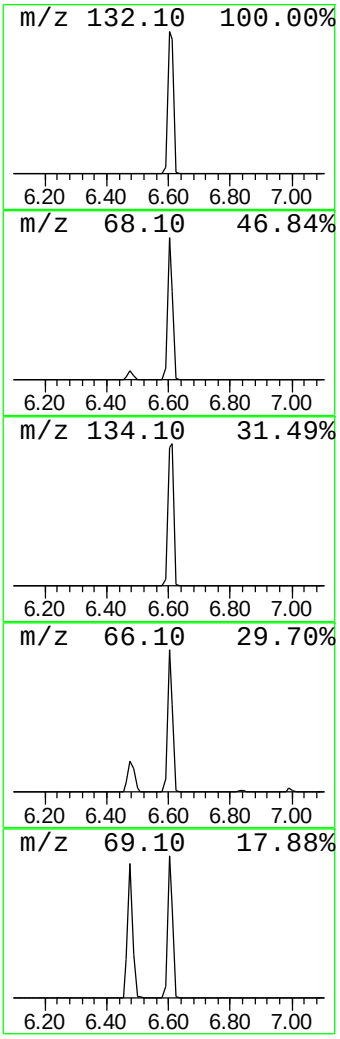
Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	84.09 ng	3854750	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CLP-S-04(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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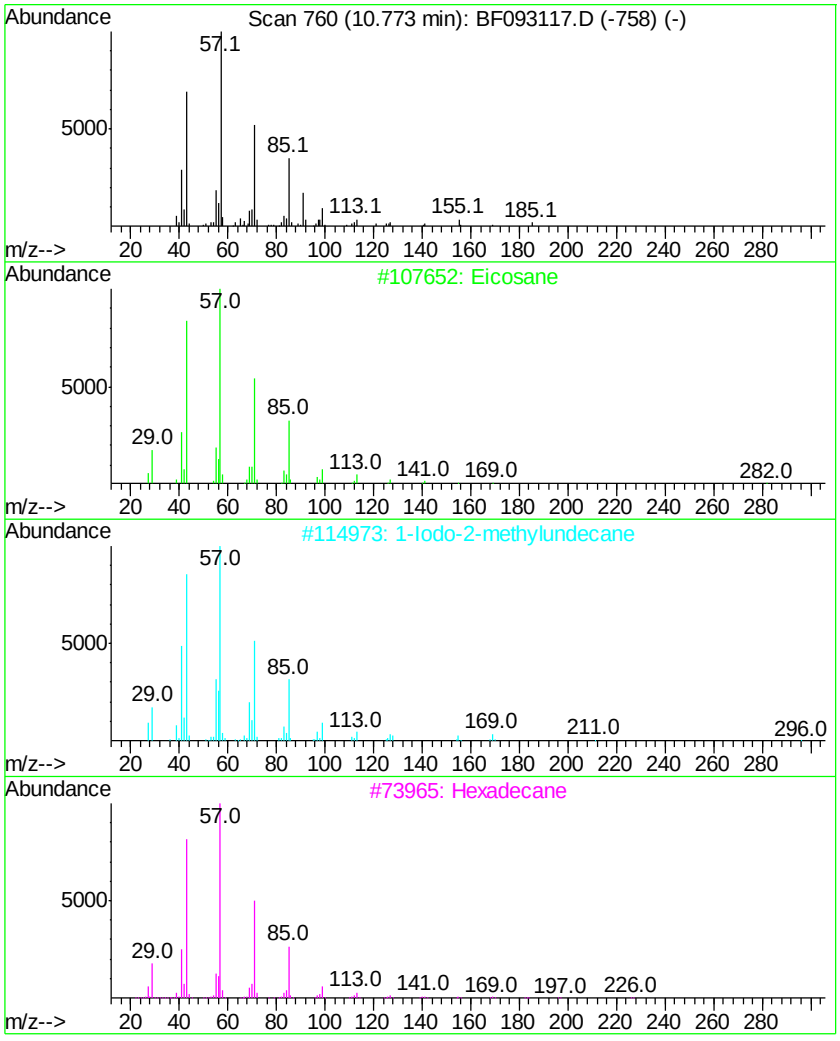
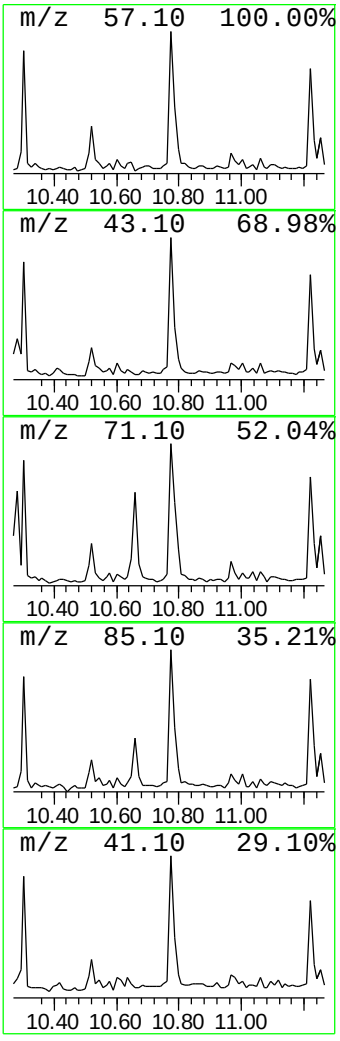
Peak Number 4 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.91 ng	212942	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	80
3	Hexadecane	226	C16H34	000544-76-3	80
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
5	Pentadecane	212	C15H32	000629-62-9	80





Library Search Compound Report

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Sample : I1954-02
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Instrument : BNA_F
ClientSampleId : CLP-S-04(5-10)

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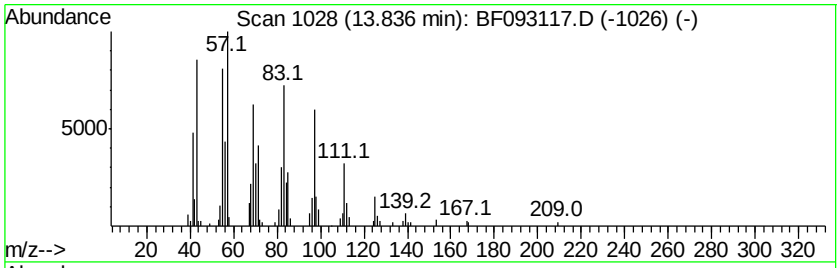
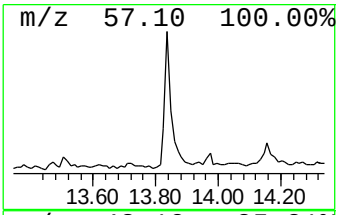
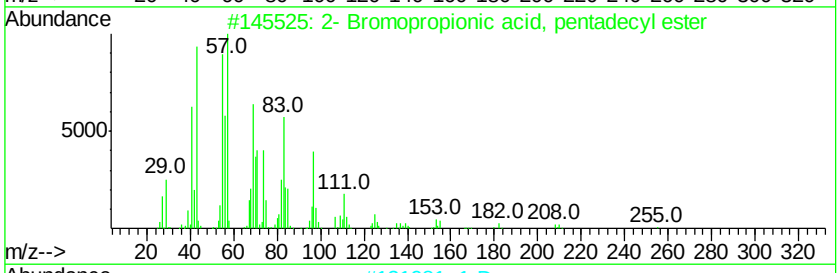
Peak Number 5 2- Bromopropionic acid, pen... Concentration Rank 4

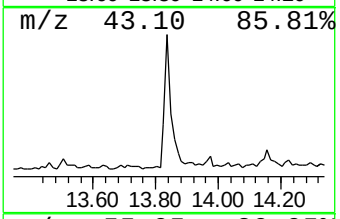
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	3.44 ng	233054	Chrysene-d12	14.00

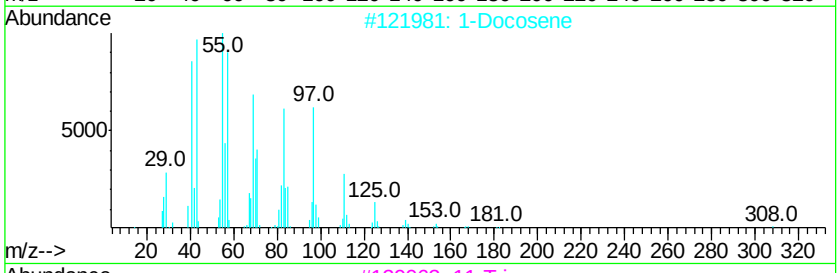
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
2	1-Docosene	308	C22H44	001599-67-3	91
3	11-Tricosene	322	C23H46	052078-56-5	91
4	1-Tetracosanol	354	C24H50O	000506-51-4	91
5	1-Nonadecene	266	C19H38	018435-45-5	91

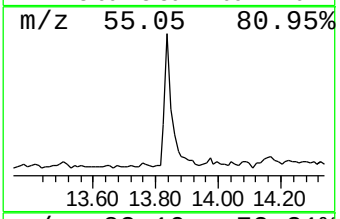


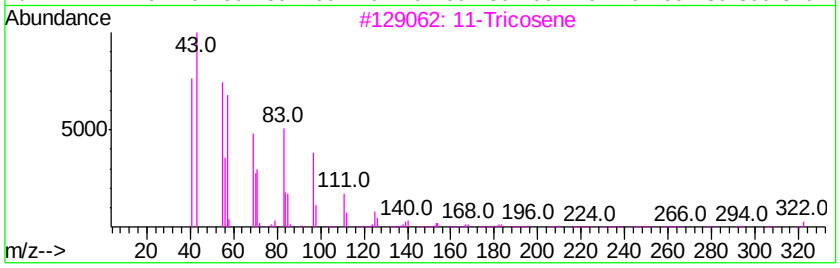


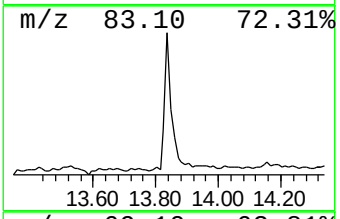


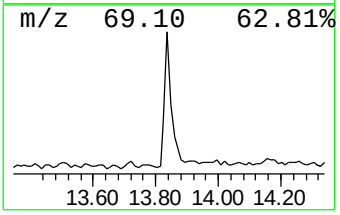












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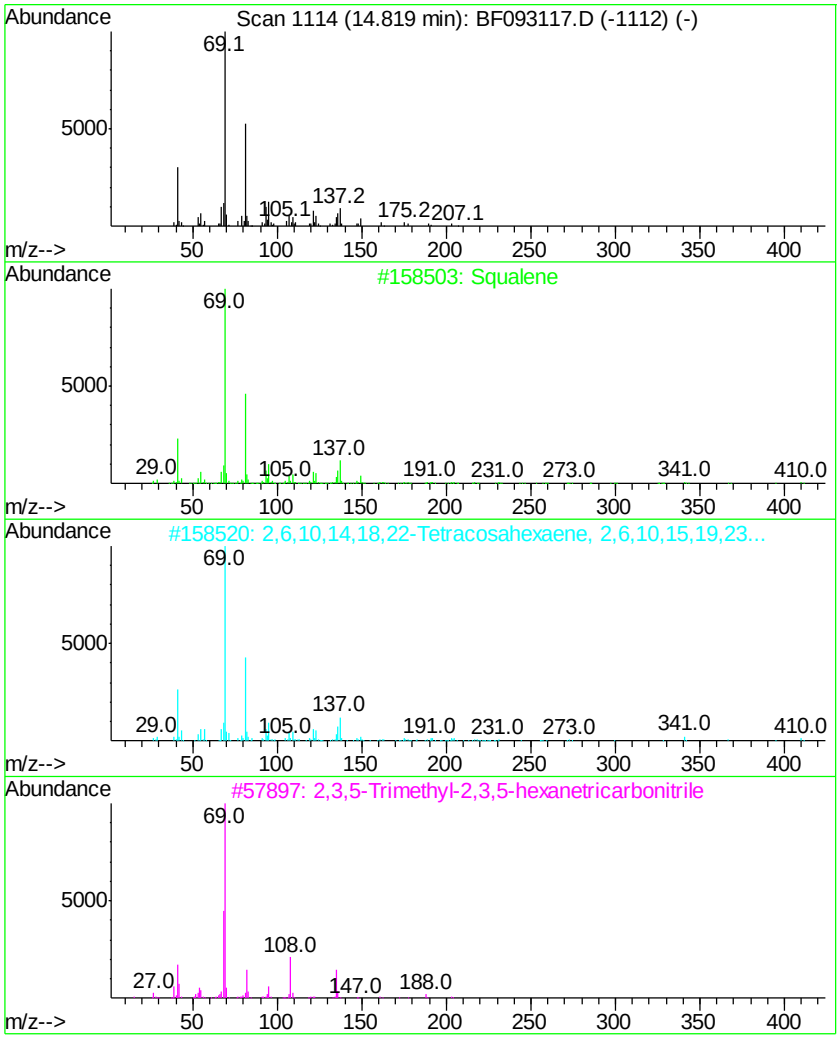
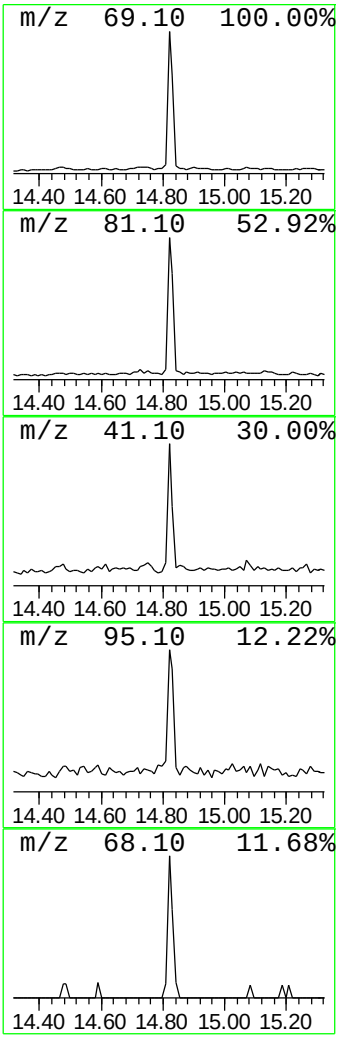
****

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.56 ng	133520	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	86
3	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58
5	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50





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...	5.01	36.5	ng	1672380	1	6.84	916784	20.0
unknown6.60	6.60	84.1	ng	3854750	1	6.84	916784	20.0
Eicosane	10.77	2.9	ng	212942	4	11.36	1464950	20.0
2- Bromopropionic...	13.84	3.4	ng	233054	5	14.00	1355560	20.0
Squalene	14.82	2.6	ng	133520	6	15.41	1042420	20.0