LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108922.D
Acq On : 11 Sep 2018 4:52
Operator : JU/SJ
Sample : J4830-12
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-B

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-BF090518.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	4.925	436	440	449	rVB	136175	150731	3.43%	0.538%
2	5.342	507	511	515	rBV	1557085	1482993	33.72%	5.291%
3	6.366	681	685	695	rVB	1275518	1062937	24.17%	3.792%
4	6.507	704	709	712	rBV	2899354	2569574	58.43%	9.168%
5	6.736	745	748	752	rBV	1155005	920388	20.93%	3.284%
6	6.895	771	775	779	rBV	3795878	3488558	79.33%	12.446%
7	7.301	838	844	847	rBV	2887007	2768843	62.97%	9.878%
8	8.019	962	966	969	rBV	1331951	1044464	23.75%	3.726%
9	9.095	1145	1149	1152	rBV	4952894	4397421	100.00%	15.689%
10	9.483	1212	1215	1227	rBV	511491	400295	9.10%	1.428%
11	9.766	1260	1263	1267	rBV	1108530	1002761	22.80%	3.578%
12	10.448	1376	1379	1382	rBV	146994	107544	2.45%	0.384%
13	10.554	1393	1397	1409	rBV	1583831	1530972	34.82%	5.462%
14	11.242	1511	1514	1518	rBV	967576	877863	19.96%	3.132%
15	12.830	1779	1784	1787	rBV	4286301	3865392	87.90%	13.791%
16	13.742	1935	1939	1949	rBV2	52616	92491	2.10%	0.330%
17	13.871	1957	1961	1965	rBV	1207550	1066196	24.25%	3.804%
18	14.724	2103	2106	2110	rVB	228204	211488	4.81%	0.755%
19	14.977	2146	2149	2154	rVB	51166	54424	1.24%	0.194%
20	15.277	2196	2200	2205	rBV2	619130	719711	16.37%	2.568%
21	15.336	2206	2210	2216	rVB	60700	81883	1.86%	0.292%
22	15.742	2275	2279	2284	rVB2	49002	71582	1.63%	0.255%
23	16.212	2354	2359	2364	rBV2	33787	60647	1.38%	0.216%

Sum of corrected areas: 28029158

LSC Report - Integrated Chromatogram

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Misc :
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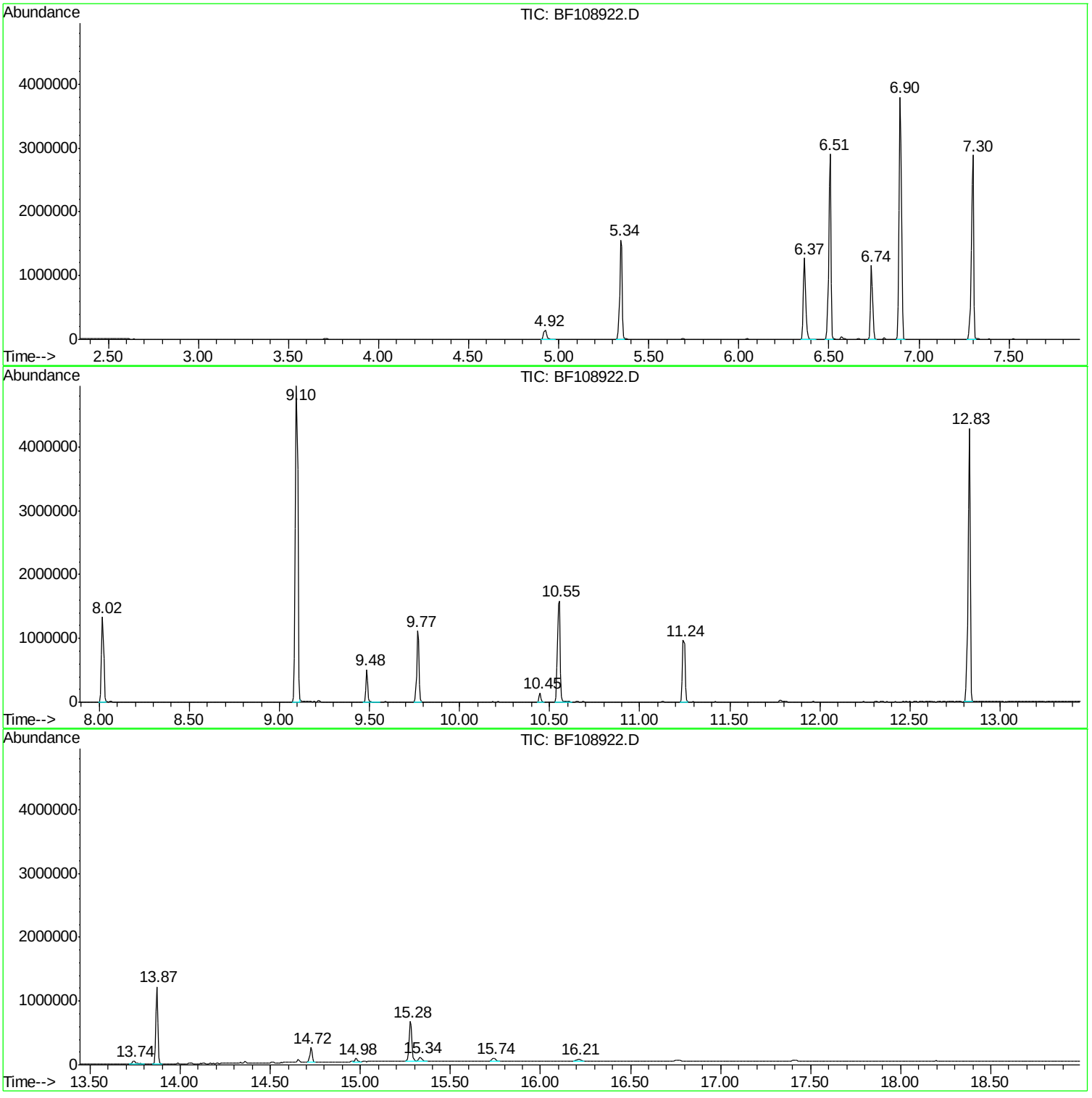
Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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ClientSampleId : 090618-DBRI-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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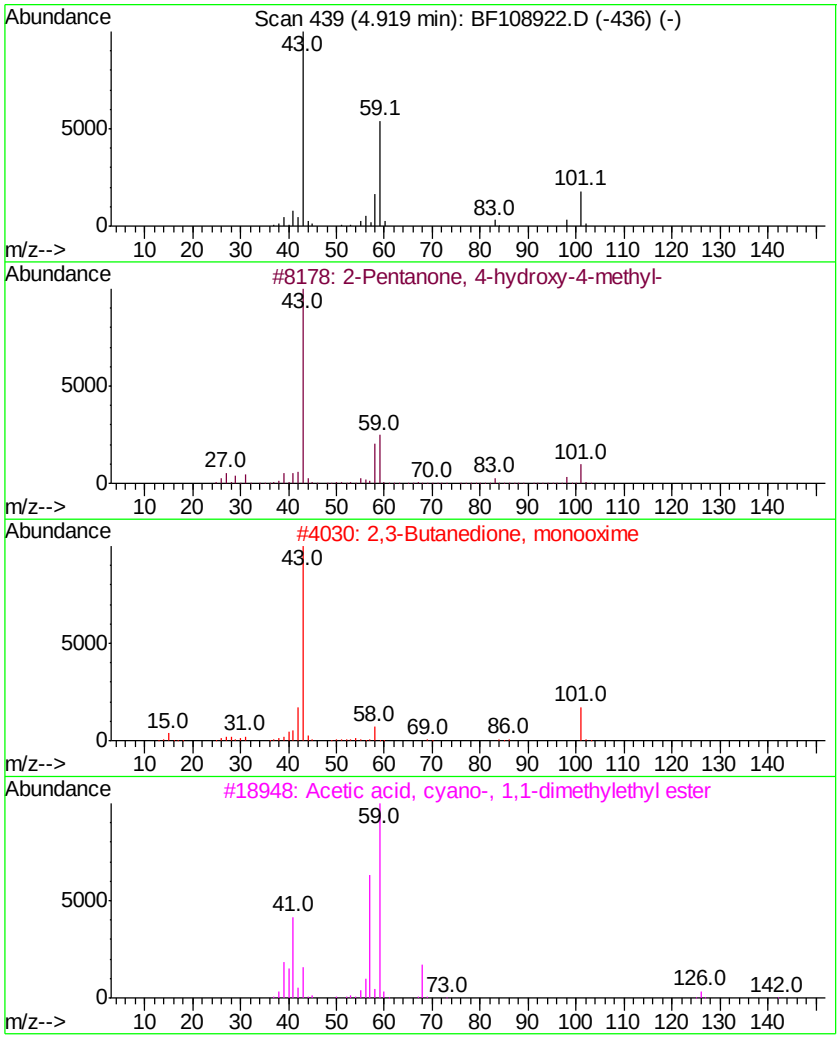
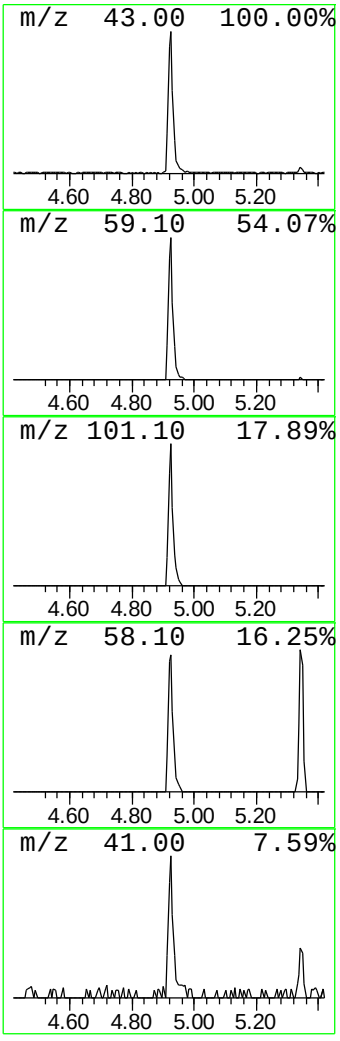
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	3.28 ng	150731	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Guanidine	59	CH5N3	000113-00-8	9





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Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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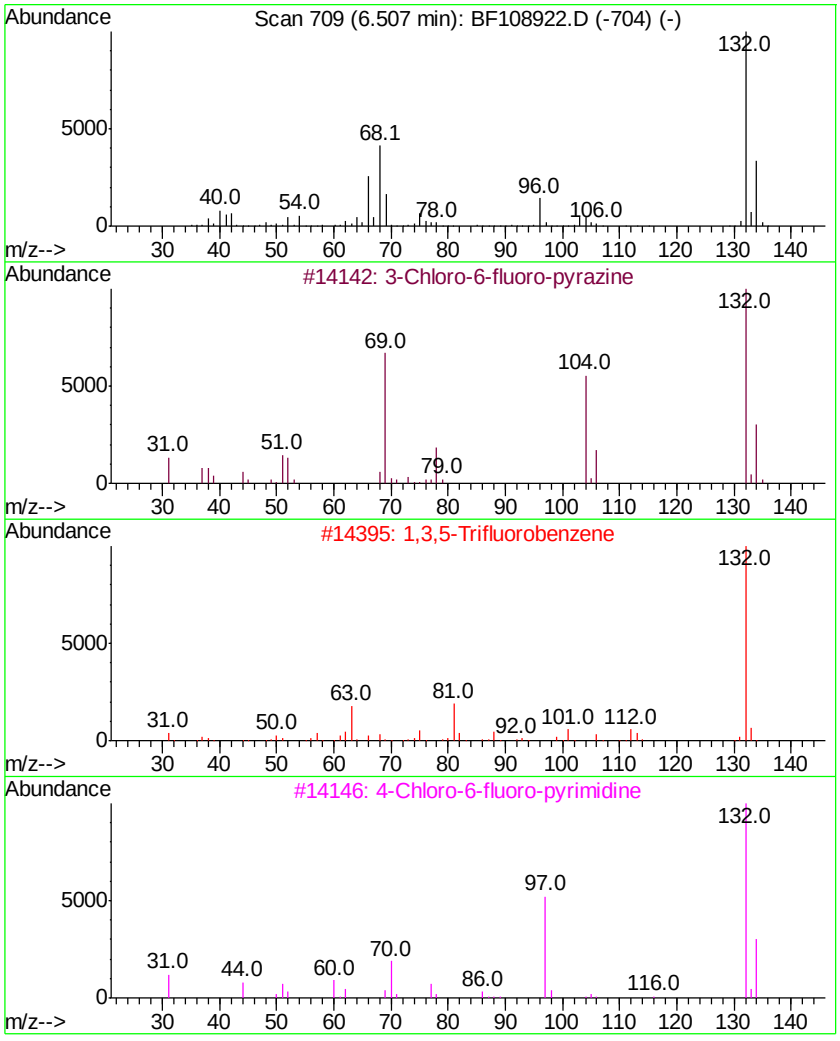
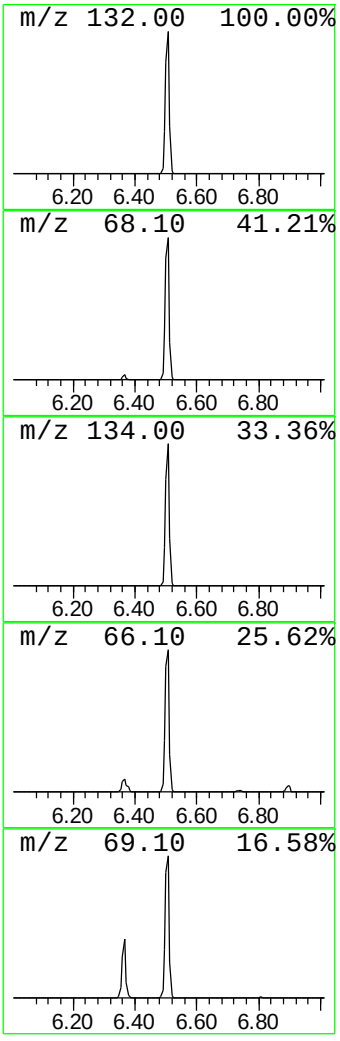
Peak Number 2 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	55.84 ng	2569570	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

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Operator : JU/SJ
Sample : J4830-12
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
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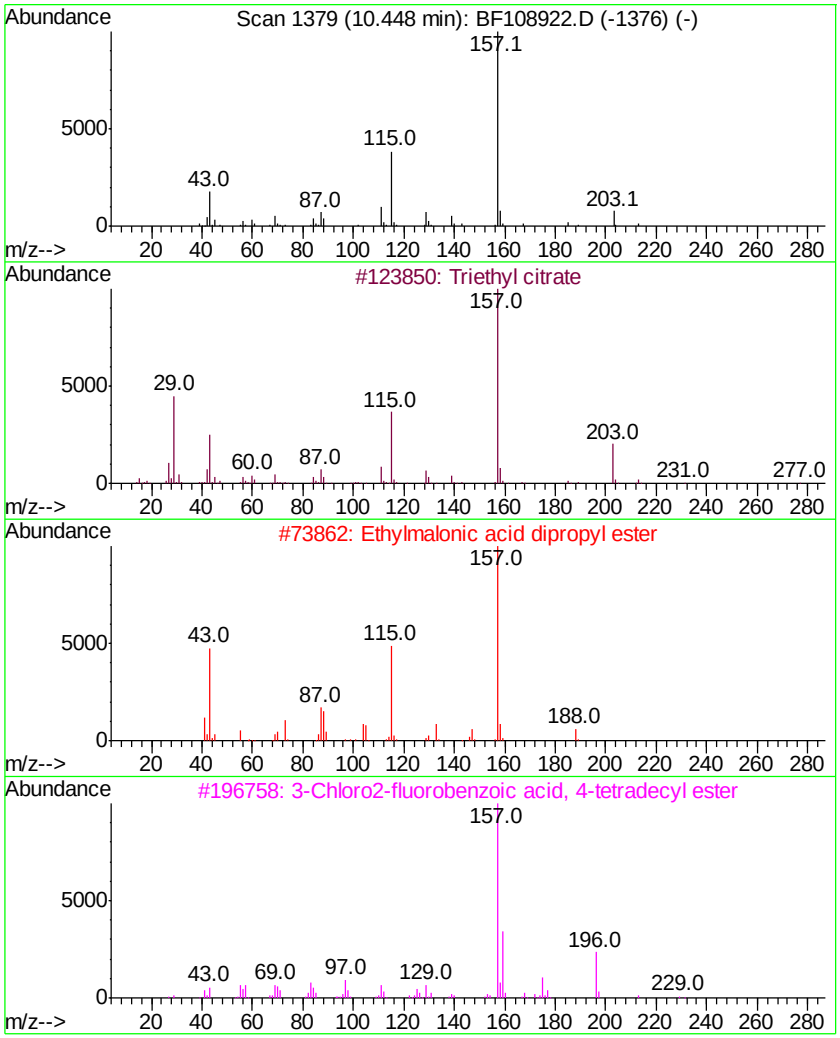
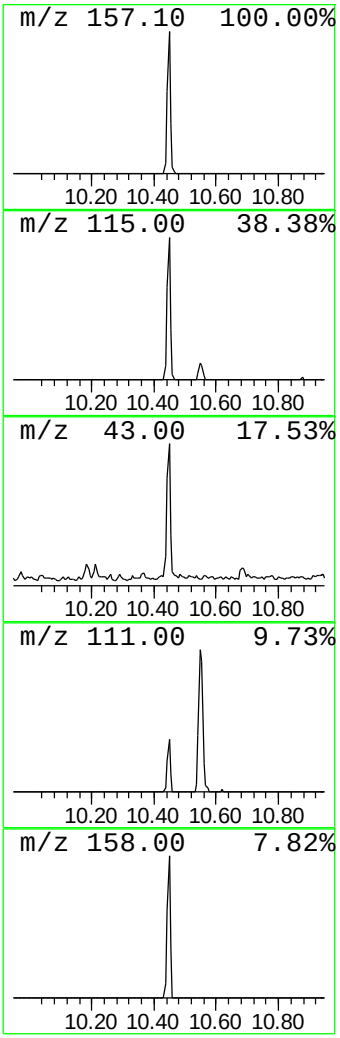
Peak Number 4 Triethyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	2.14 ng	107544	Acenaphthene-d10	9.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	90
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	40
4	3-Chloro2-fluorobenzoic acid, 6-...	370	C21H32ClFO2	1000338-64-9	40
5	Piperazine-1-carboxylic acid, 4-...	396	C14H18Cl2N2O5S	1000303-80-3	38





Library Search Compound Report

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Sample : J4830-12
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
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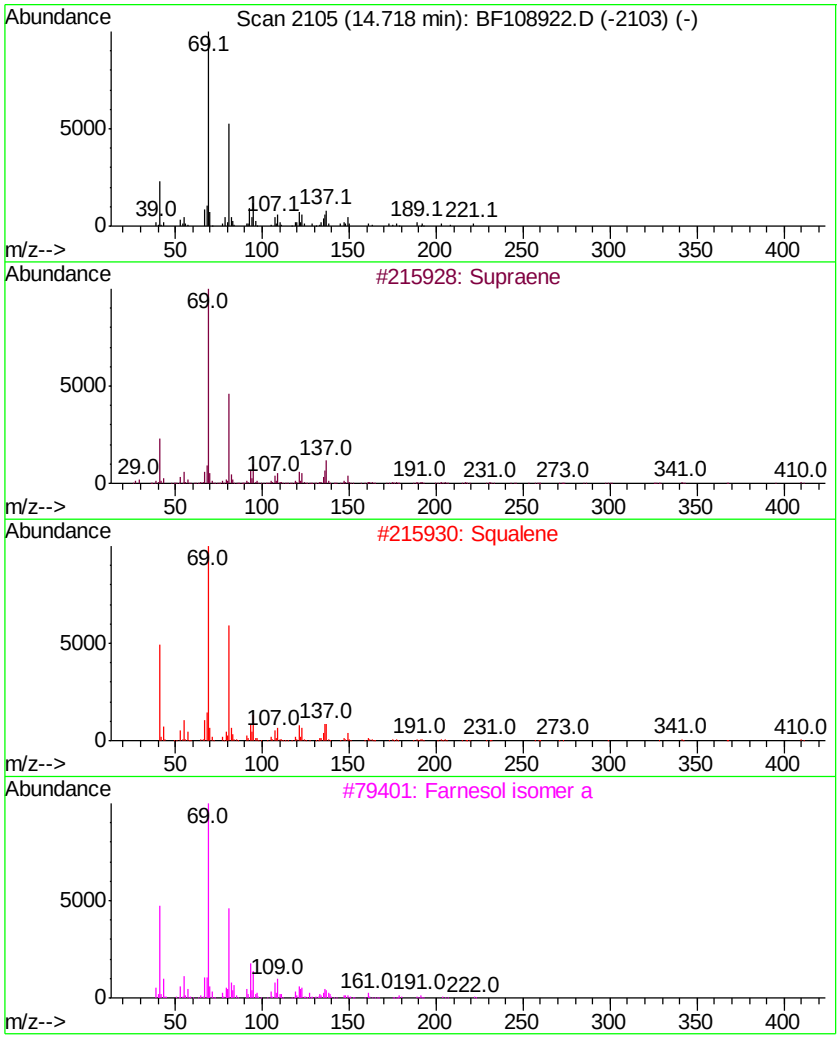
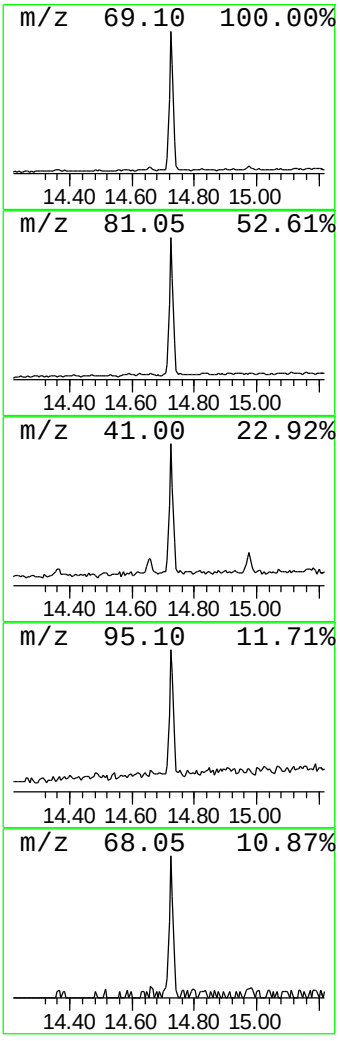
Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	5.88 ng	211488	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	Farnesol isomer a	222	C15H26O	1000108-92-4	64
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64





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Sample : J4830-12
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ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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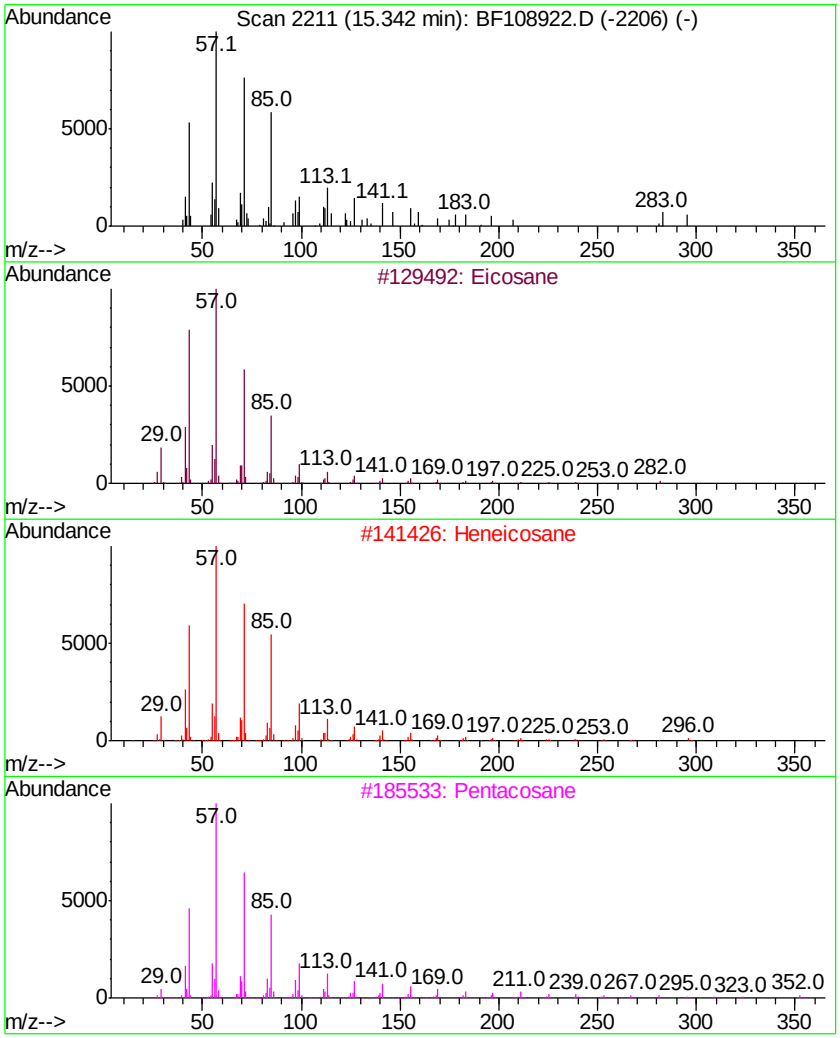
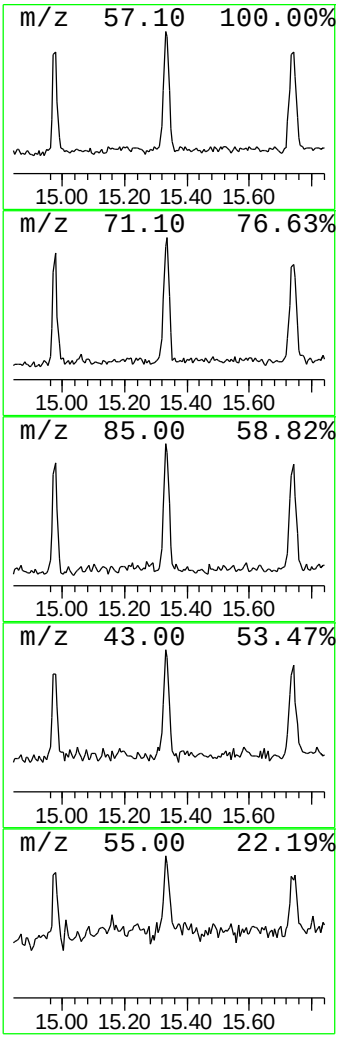
Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	2.28 ng	81883	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Pentacosane	352	C25H52	000629-99-2	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	86





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	4.92	3.3	ng	150731	1	6.74	920388	20.0
unknown6.51	6.51	55.8	ng	2569570	1	6.74	920388	20.0
Triethyl citrate	10.45	2.1	ng	107544	3	9.77	1002760	20.0
Supraene	14.72	5.9	ng	211488	6	15.28	719711	20.0
Eicosane	15.34	2.3	ng	81883	6	15.28	719711	20.0