LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099542.D
Acq On : 16 Oct 2017 14:12
Operator : SJ/JU
Sample : I5875-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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	5.057	502	505	516	rBV	47105	56935	1.90%	0.445%
2	5.463	571	574	593	rVB	281060	314636	10.51%	2.458%
3	6.475	743	746	753	rBV	237566	267491	8.94%	2.090%
4	6.610	766	769	775	rBV	503262	467920	15.64%	3.656%
5	6.845	805	809	815	rBV	646250	595943	19.92%	4.656%
6	6.916	815	821	824	rVV	581513	499837	16.70%	3.905%
7	6.951	824	827	831	rVV	164730	124136	4.15%	0.970%
8	6.998	831	835	845	rVB	603094	503367	16.82%	3.933%
9	7.404	901	904	915	rVB	428176	381153	12.74%	2.978%
10	7.516	918	923	929	rBV	86271	105676	3.53%	0.826%
11	7.857	975	981	984	rBV	2769718	2992278	100.00%	23.378%
12	7.957	995	998	1001	rVB	183156	145452	4.86%	1.136%
13	8.128	1023	1027	1029	rBV	904936	891315	29.79%	6.964%
14	8.145	1029	1030	1034	rVB	502325	292304	9.77%	2.284%
15	8.504	1079	1091	1093	rBV4	27188	48924	1.64%	0.382%
16	8.839	1144	1148	1155	rBV	259629	263253	8.80%	2.057%
17	8.939	1161	1165	1168	rBV	136147	122490	4.09%	0.957%
18	9.198	1205	1209	1212	rBV	812426	674780	22.55%	5.272%
19	9.469	1250	1255	1259	rBV2	31725	42744	1.43%	0.334%
20	9.539	1263	1267	1269	rVV	53363	56702	1.89%	0.443%
21	9.592	1273	1276	1282	rVB	84044	69431	2.32%	0.542%
22	9.880	1321	1325	1333	rVB	949600	822119	27.47%	6.423%
23	10.022	1346	1349	1353	rBV	29313	31274	1.05%	0.244%
24	10.298	1390	1396	1399	rBV2	46755	40642	1.36%	0.318%
25	10.669	1456	1459	1468	rBV	280990	252824	8.45%	1.975%
26	10.769	1474	1476	1481	rBV	47160	50518	1.69%	0.395%
27	11.369	1574	1578	1581	rBV	824256	672796	22.48%	5.256%
28	12.945	1843	1846	1850	rBV	512233	442485	14.79%	3.457%
29	13.839	1994	1998	2007	rVB3	43871	65803	2.20%	0.514%
30	13.974	2018	2021	2024	rVB	54951	43272	1.45%	0.338%
31	14.010	2024	2027	2031	rBV	588264	525483	17.56%	4.106%
32	15.092	2208	2211	2215	rVB2	28699	31337	1.05%	0.245%
33	15.486	2272	2278	2284	rBV	466782	597426	19.97%	4.668%
34	15.898	2344	2348	2354	rVB2	31528	46500	1.55%	0.363%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I5875-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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

35	16.398	2428	2433	2439	rBV2	37271	60008	2.01%	0.469%
36	16.980	2527	2532	2539	rVB2	31863	62493	2.09%	0.488%
37	17.680	2644	2651	2661	rVB3	34214	82993	2.77%	0.648%
38	18.492	2783	2789	2798	rBV5	19187	54743	1.83%	0.428%

Sum of corrected areas: 12799483

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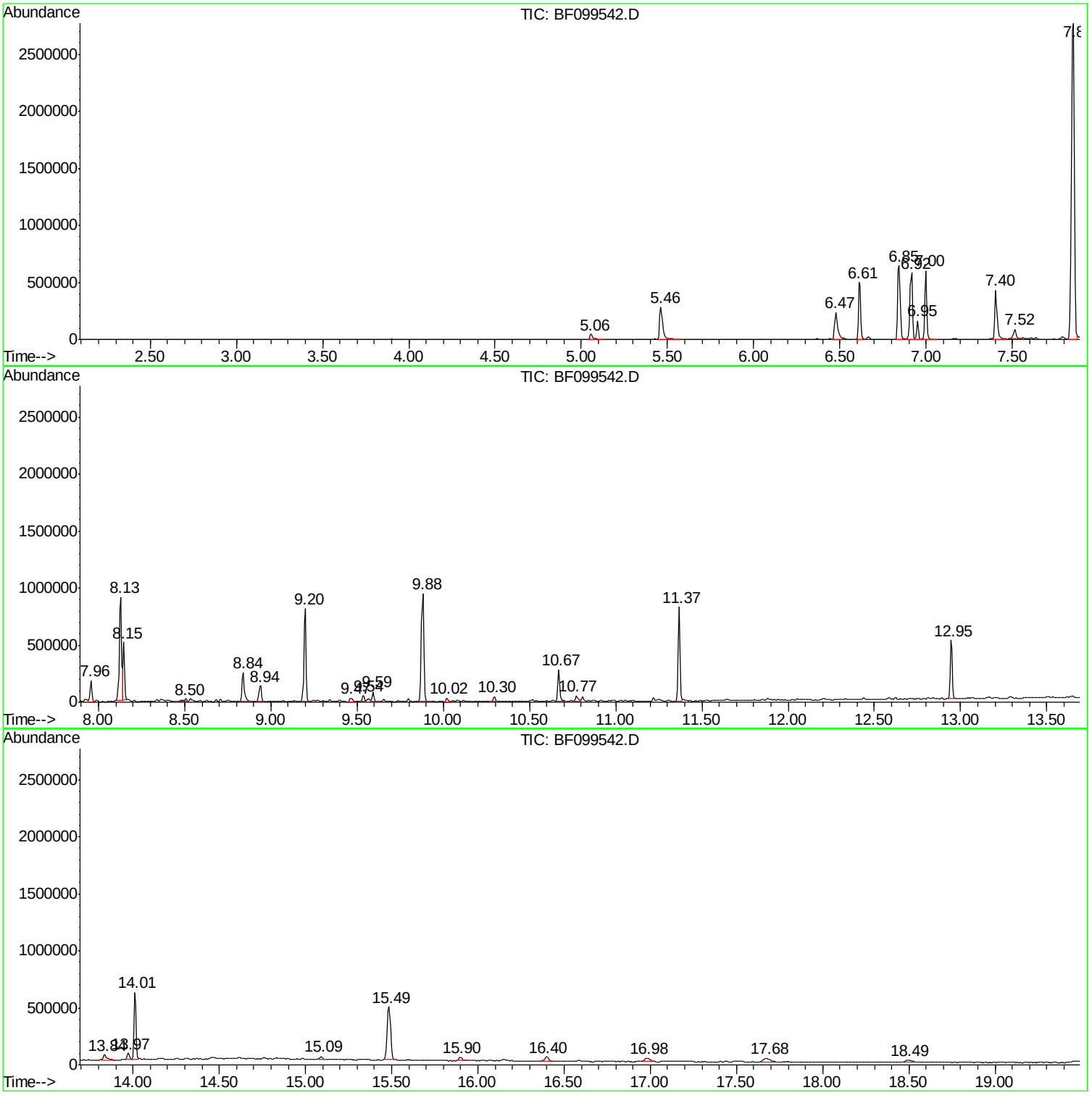
Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099542.D
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Operator : SJ/JU
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Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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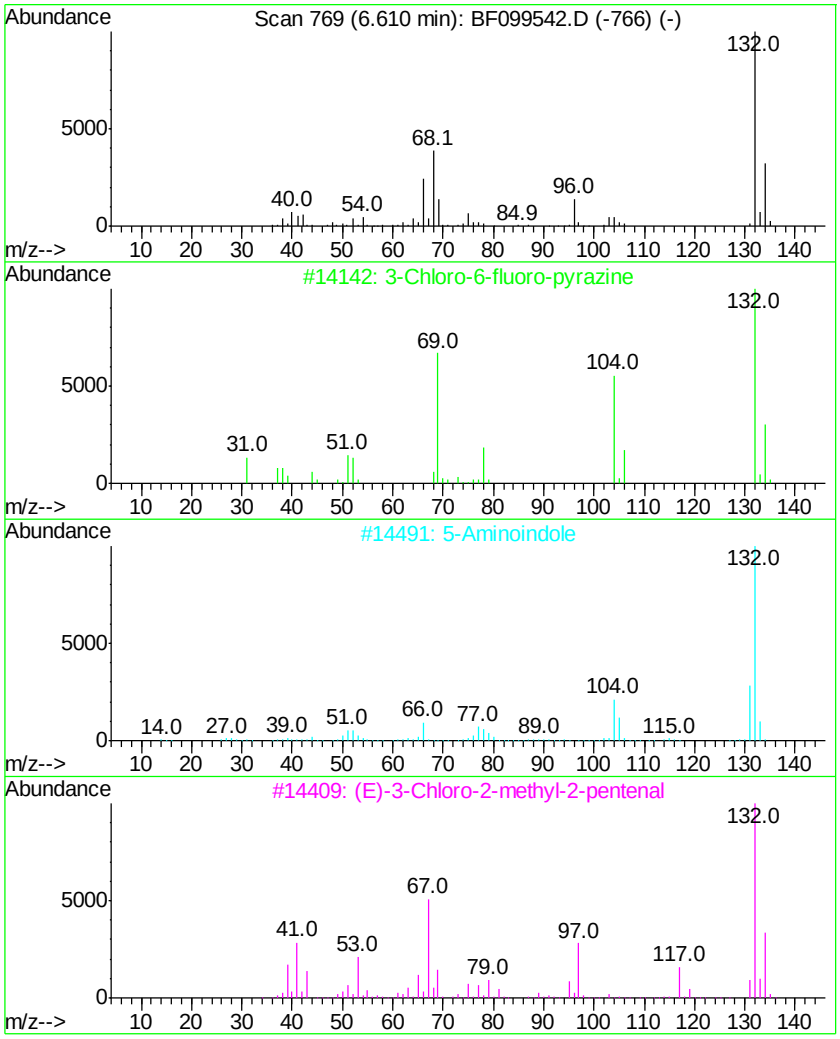
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

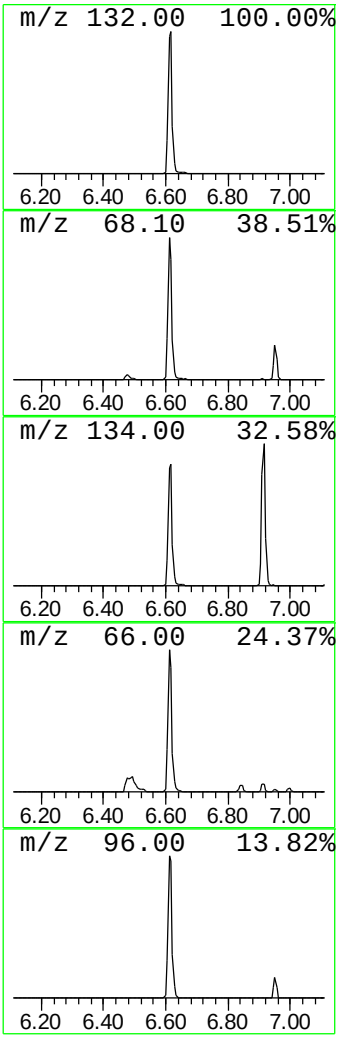
****

Peak Number 1 unknown6.61 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	15.70 ng	467920	1,4-Dichlorobenzene-d4	6.85

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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099542.D
Acq On : 16 Oct 2017 14:12
Operator : SJ/JU
Sample : I5875-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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

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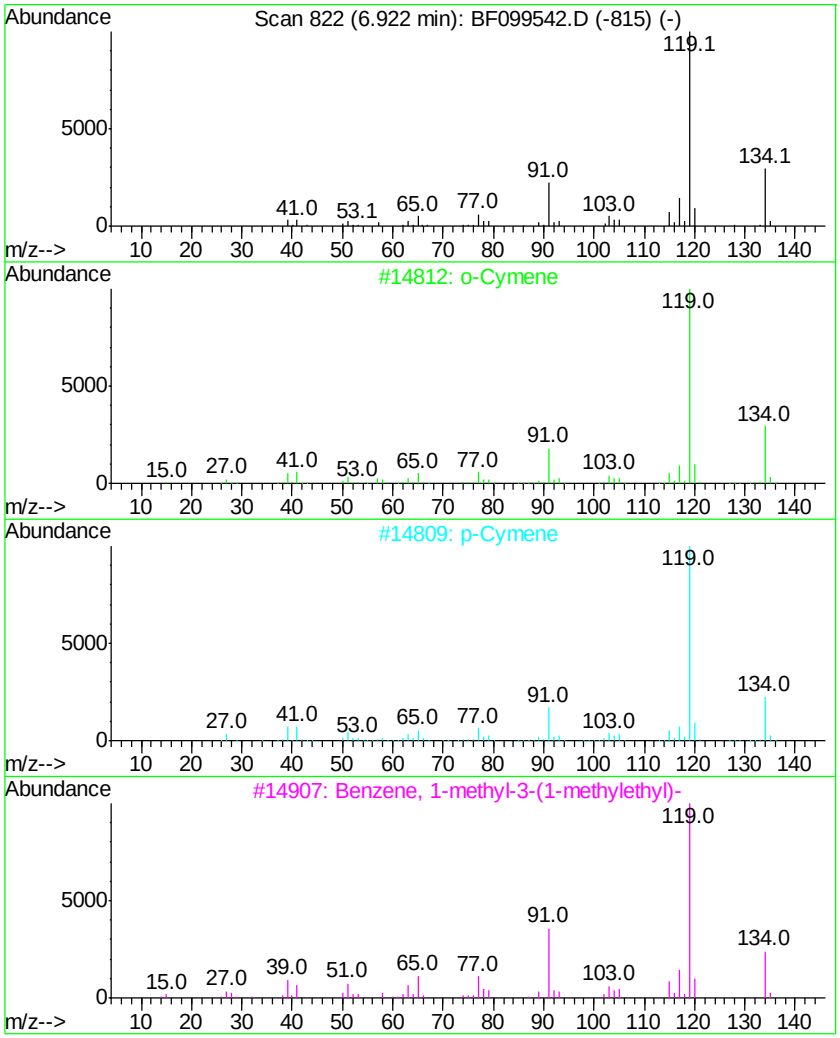
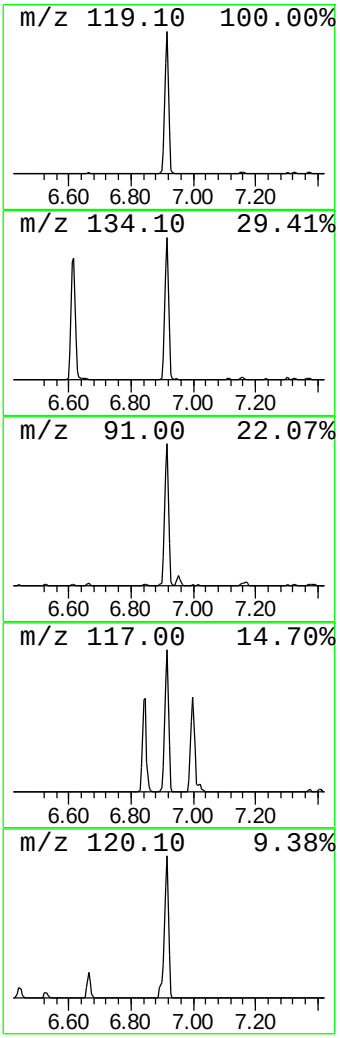
Peak Number 2 o-Cymene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	16.77 ng	499837	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	p-Cymene	134	C10H14	000099-87-6	97
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099542.D
Acq On : 16 Oct 2017 14:12
Operator : SJ/JU
Sample : I5875-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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

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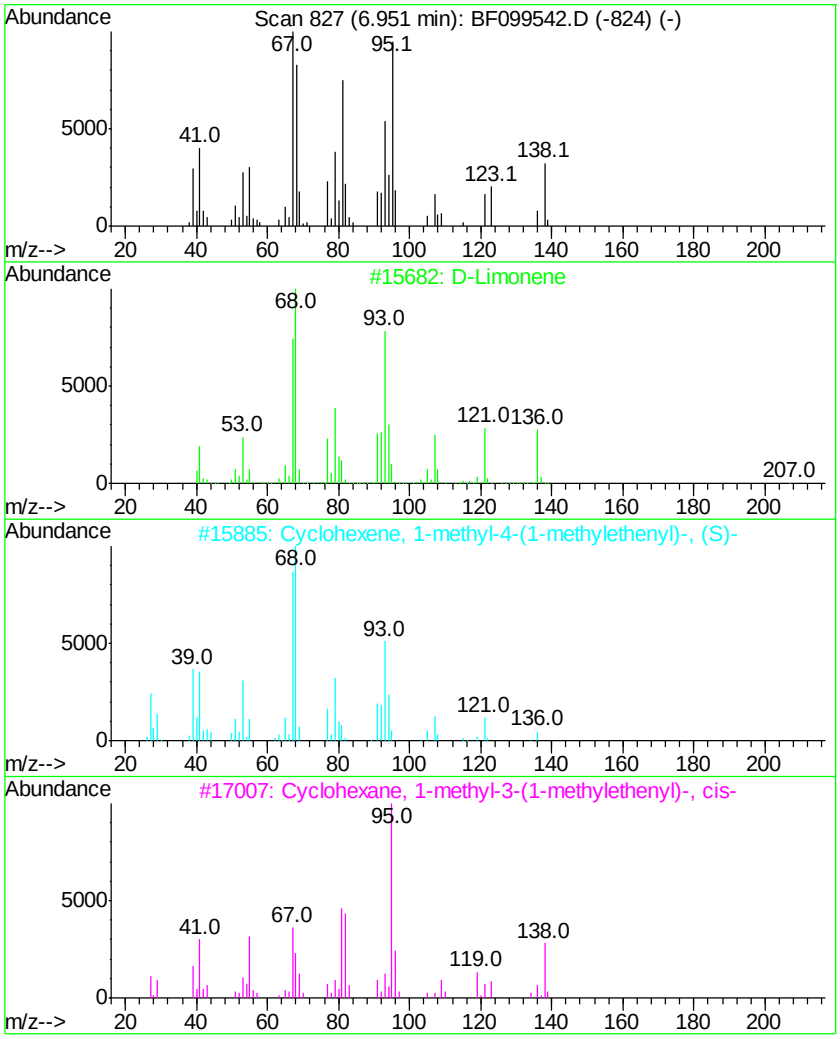
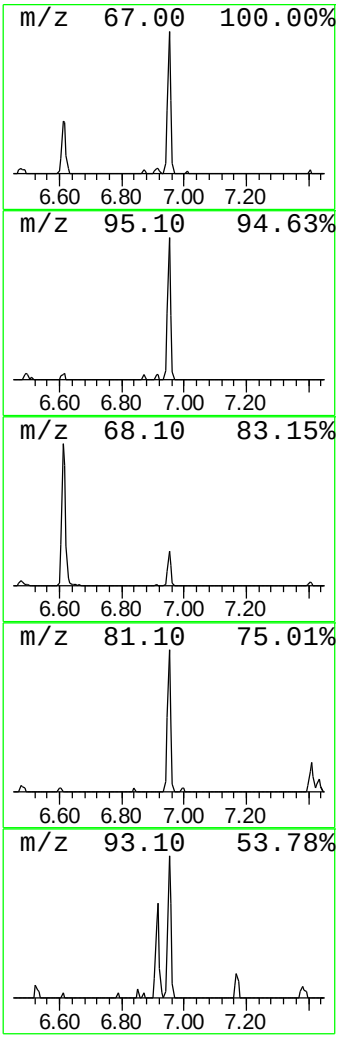
Peak Number 3 D-Limonene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	4.17 ng	124136	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	87
2	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	87
3	Cyclohexane, 1-methyl-3-(1-methy...	138	C10H18	024399-15-3	58
4	Cyclohexene, 3-methyl-6-(1-methy...	138	C10H18	005256-65-5	58
5	Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-27-2	55





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
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Operator : SJ/JU
Sample : I5875-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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

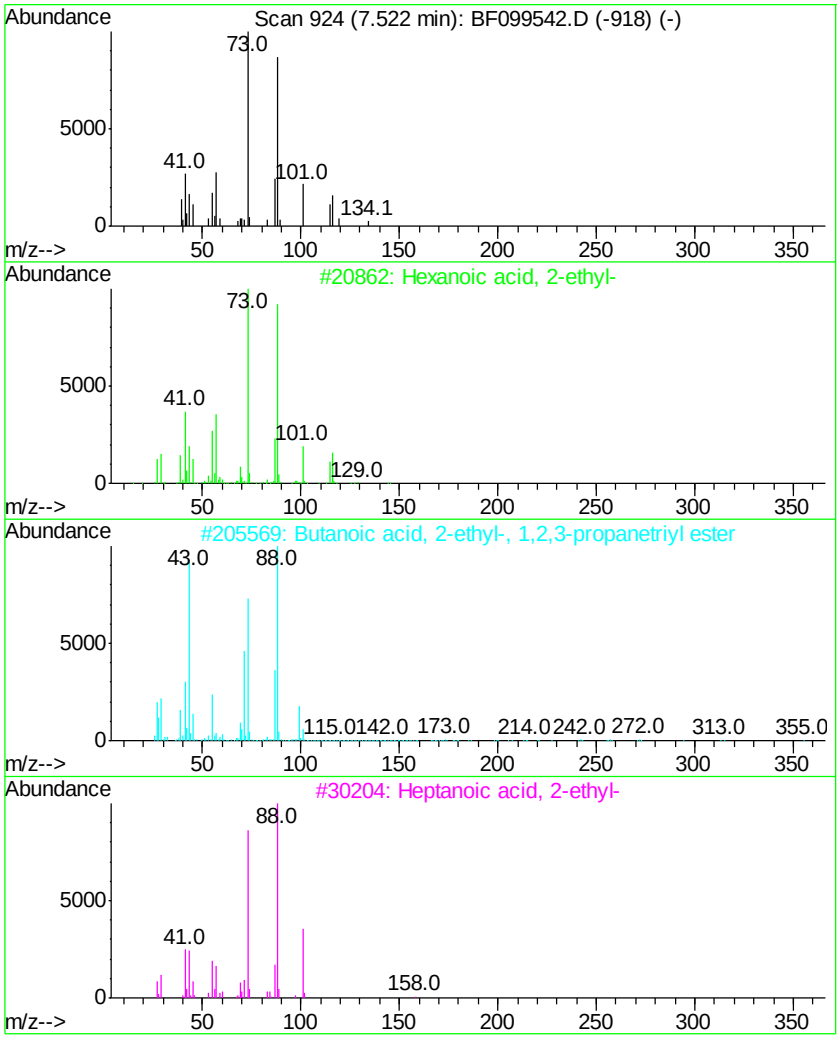
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

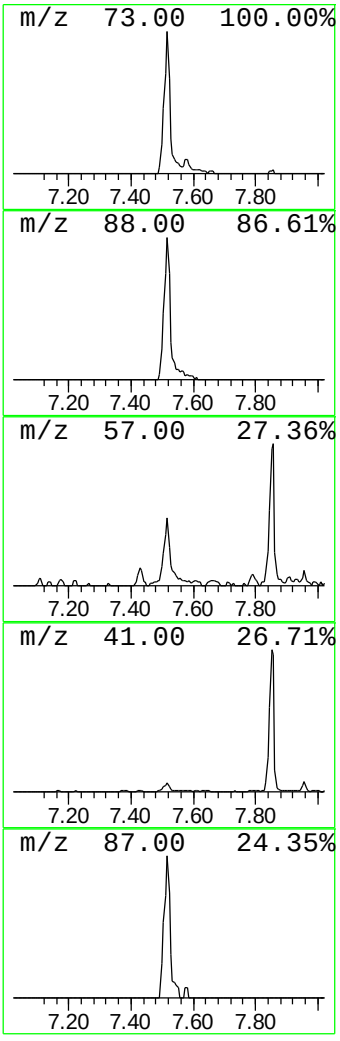
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.52	2.37 ng	105676	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	45
4	Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	40
5	1,4-Dioxane	88	C4H8O2	000123-91-1	37





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Sample : I5875-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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

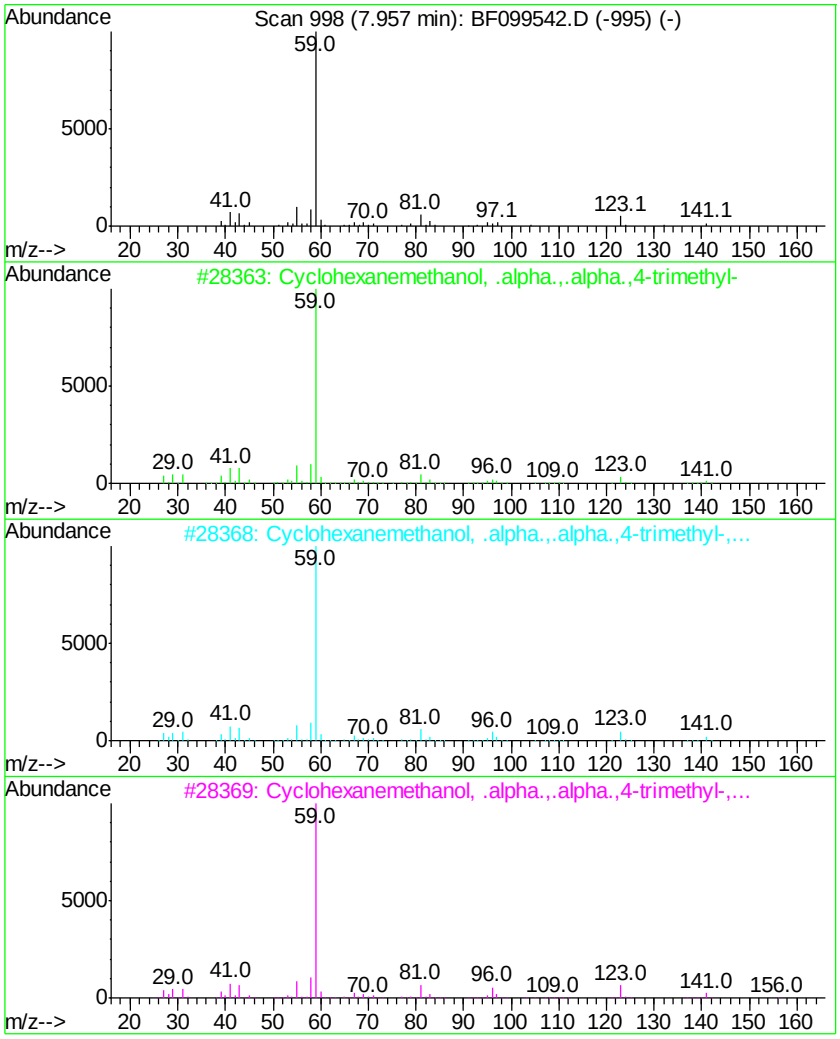
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

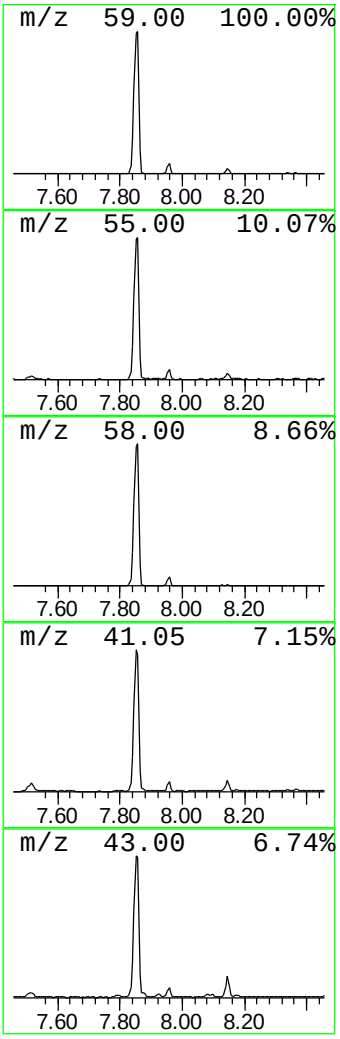
****

Peak Number 7 Cyclohexanemethanol, .alpha... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.96	3.26 ng	145452	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	83
2	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	007322-63-6	83
3	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	72
4	2,3-Dimethyl-4-penten-2-ol	114	C7H14O	019781-52-3	64
5	Butane, 2-methoxy-3-methyl-	102	C6H14O	062016-49-3	50





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Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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

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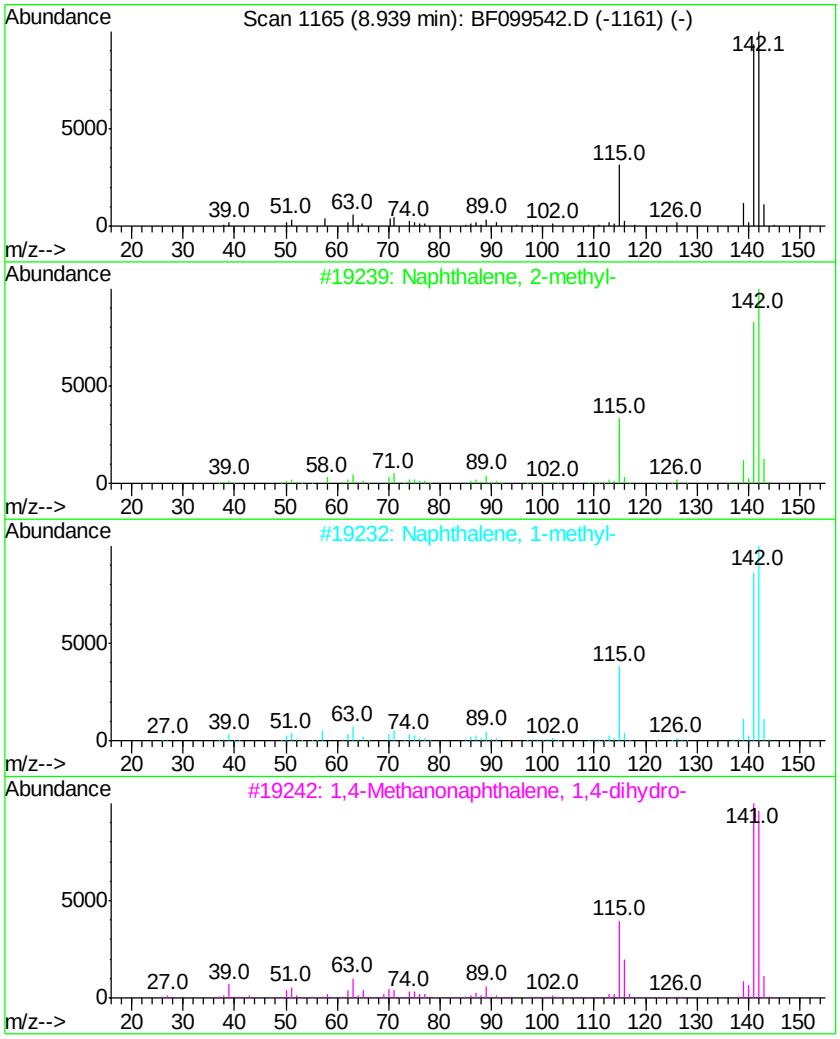
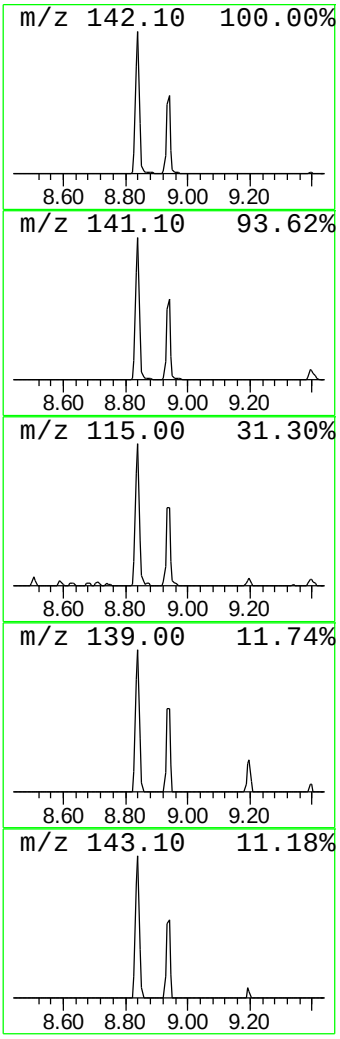
Peak Number 8 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.94	2.75 ng	122490	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	86





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Misc :
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Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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

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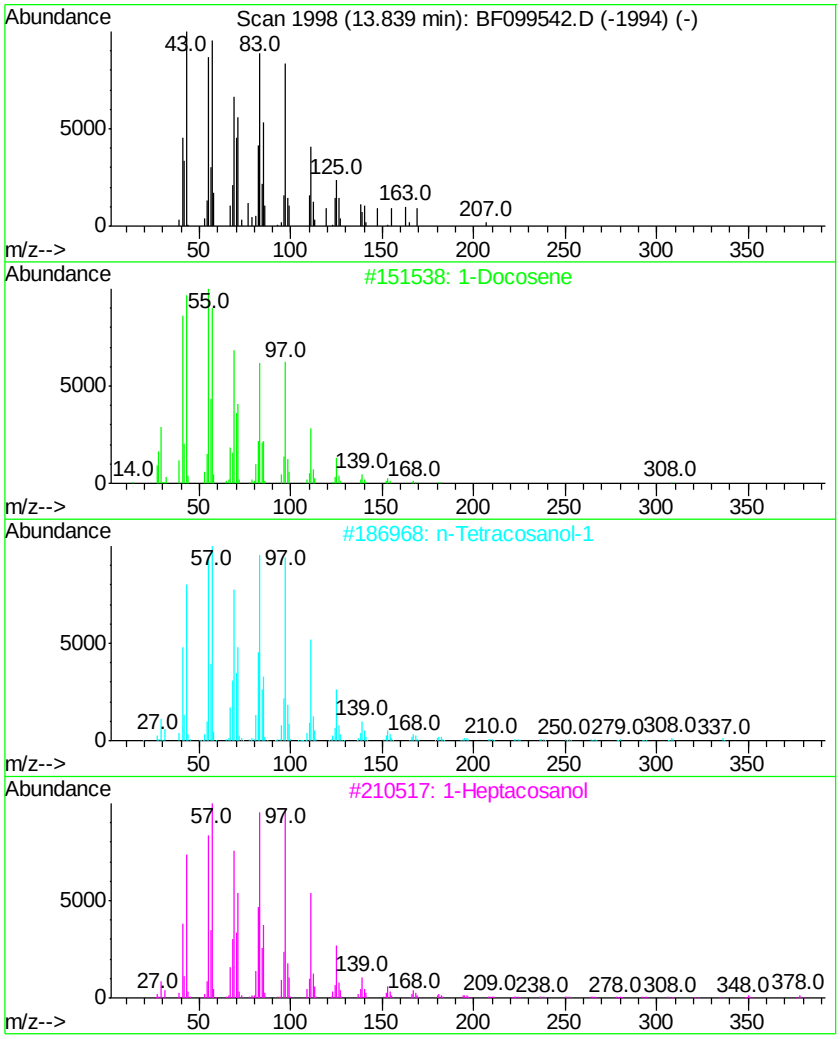
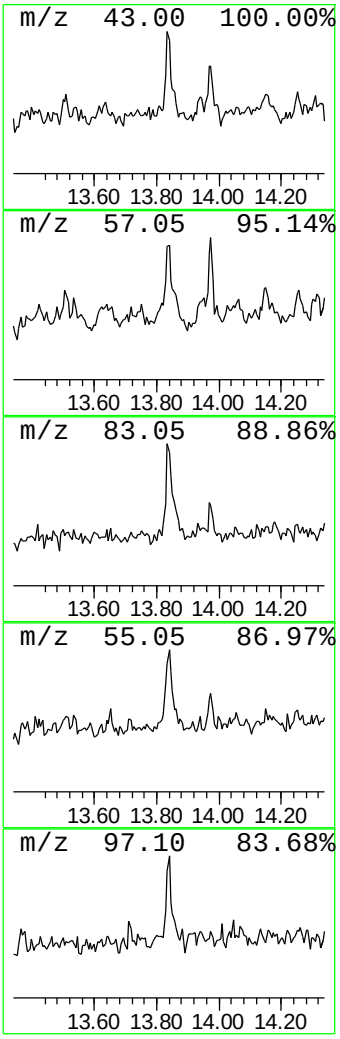
Peak Number 9 1-Docosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	2.50 ng	65803	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	83
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	81
3	1-Heptacosanol	396	C27H56O	002004-39-9	81
4	Behenic alcohol	326	C22H46O	000661-19-8	81
5	17-Pentatriacontene	491	C35H70	006971-40-0	80





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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

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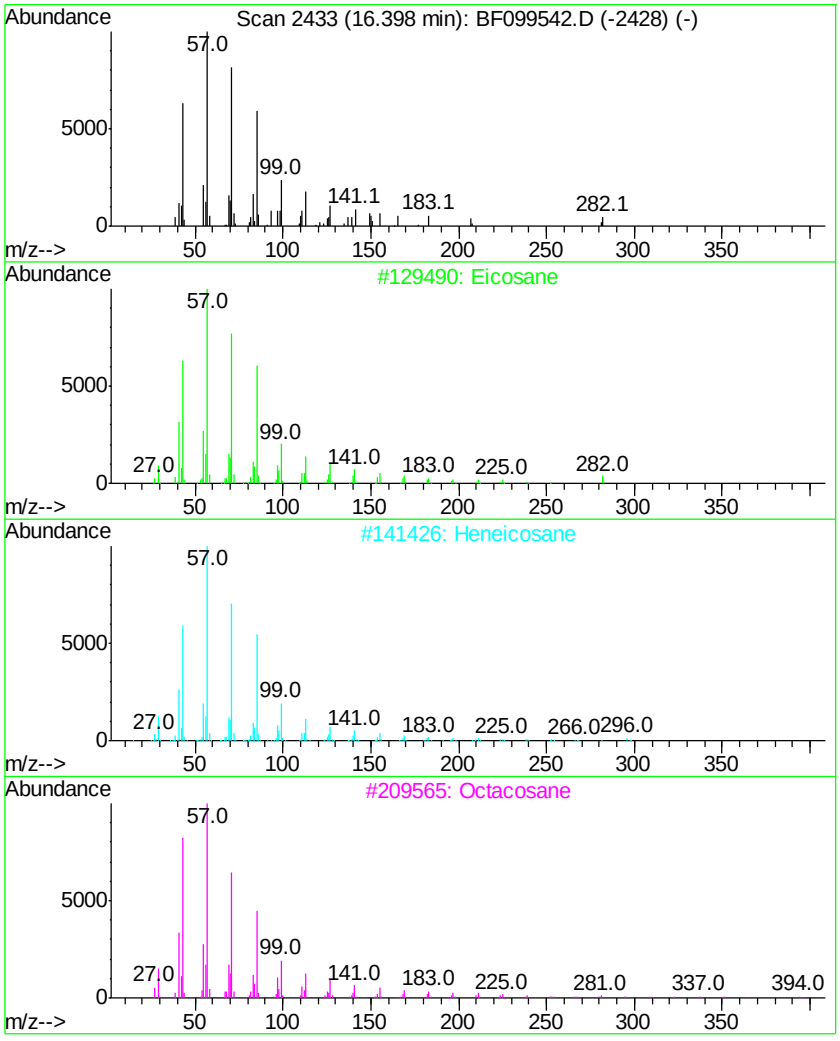
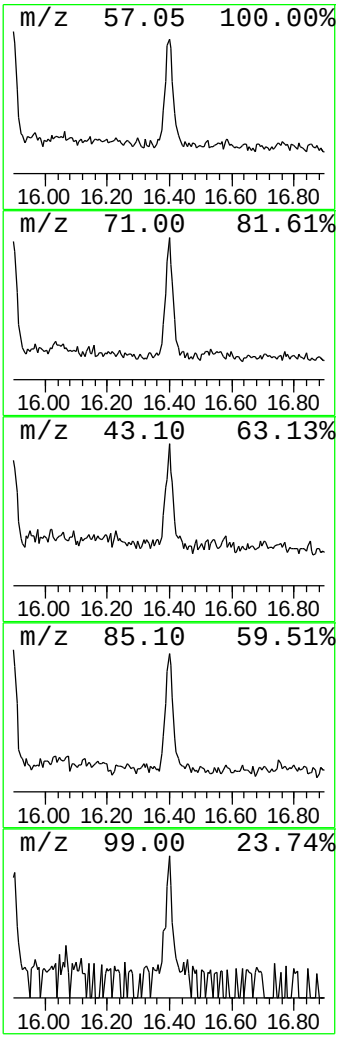
Peak Number 10 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	2.01 ng	60008	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heneicosane	296	C21H44	000629-94-7	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Heptadecane	240	C17H36	000629-78-7	86
5	Tetracosane	338	C24H50	000646-31-1	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099542.D
Acq On : 16 Oct 2017 14:12
Operator : SJ/JU
Sample : I5875-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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

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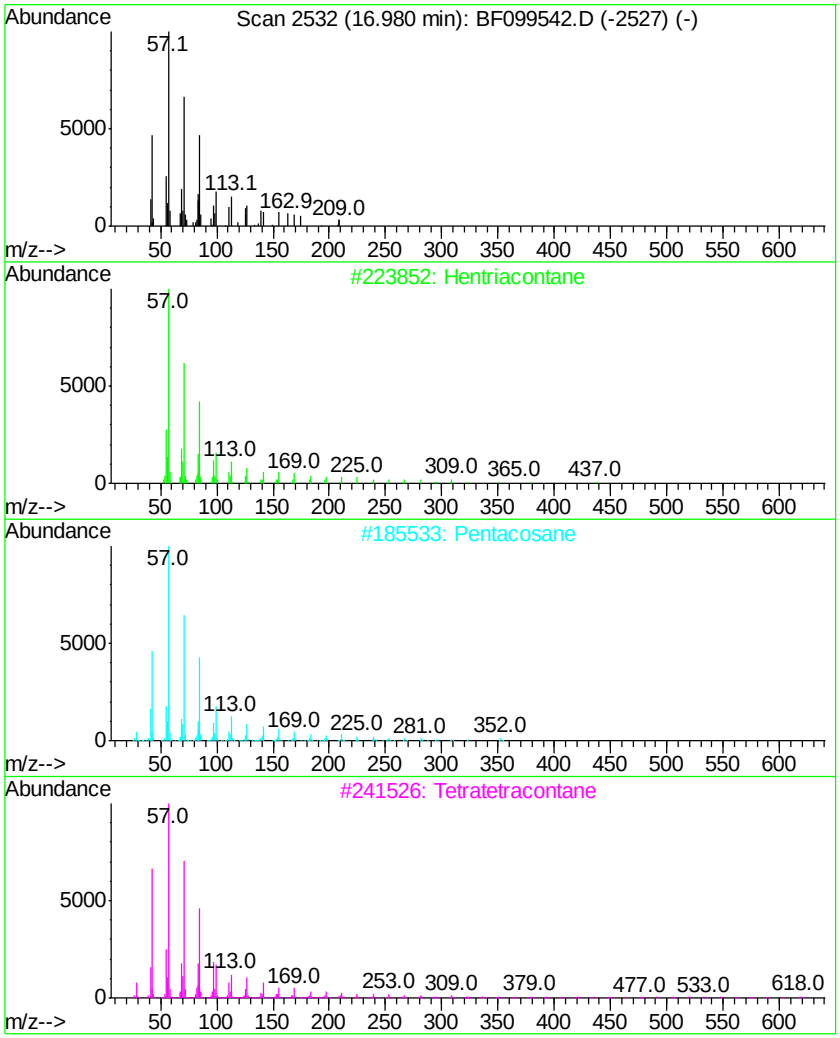
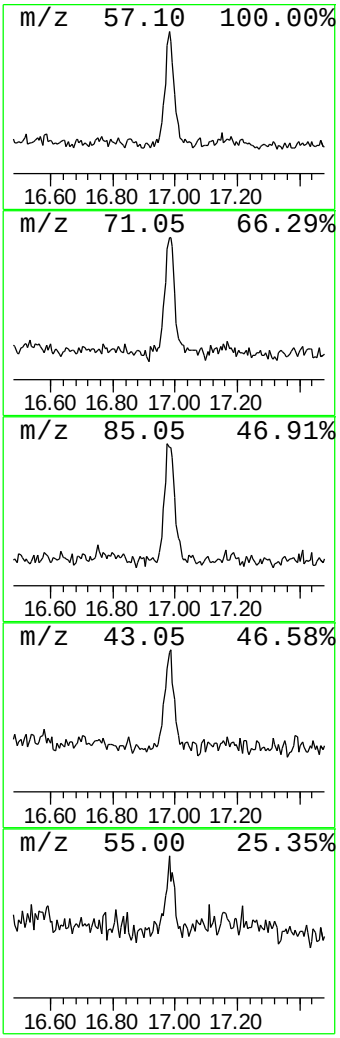
Peak Number 11 Hentriacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.98	2.09 ng	62493	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Pentacosane	352	C25H52	000629-99-2	87
3	Tetratetracontane	619	C44H90	007098-22-8	86
4	Hexacosane	366	C26H54	000630-01-3	86
5	10-Methylnonadecane	282	C20H42	056862-62-5	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099542.D
Acq On : 16 Oct 2017 14:12
Operator : SJ/JU
Sample : I5875-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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

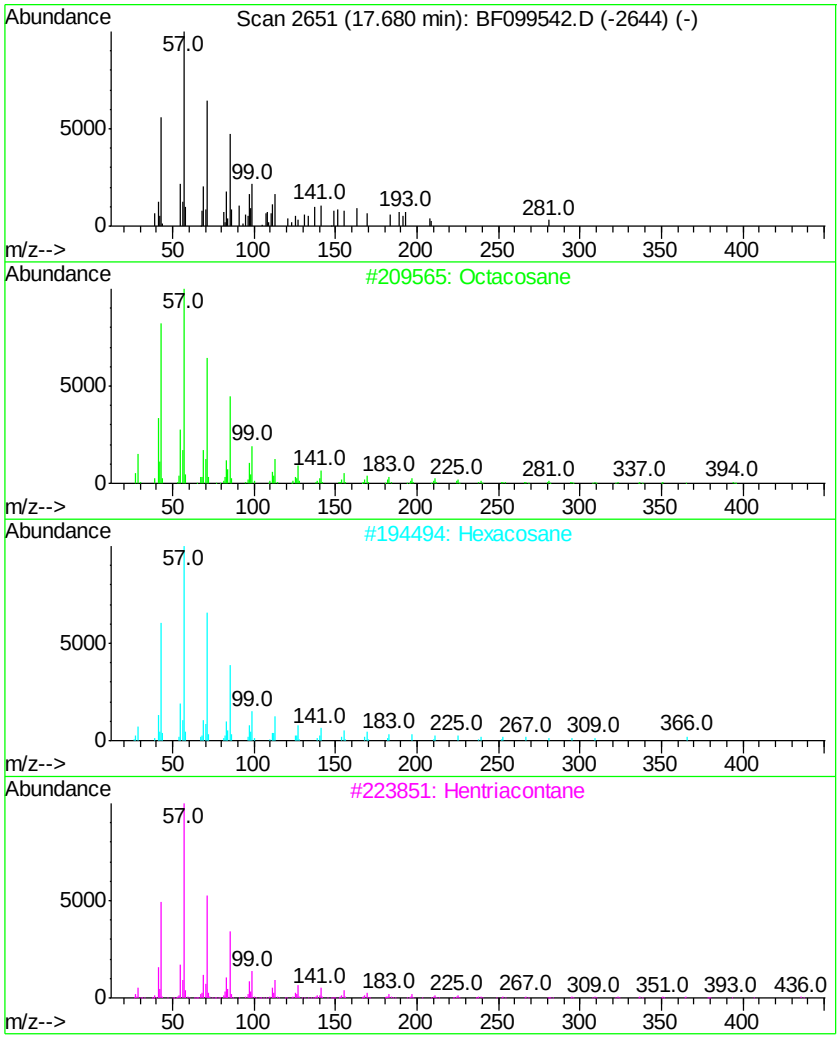
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

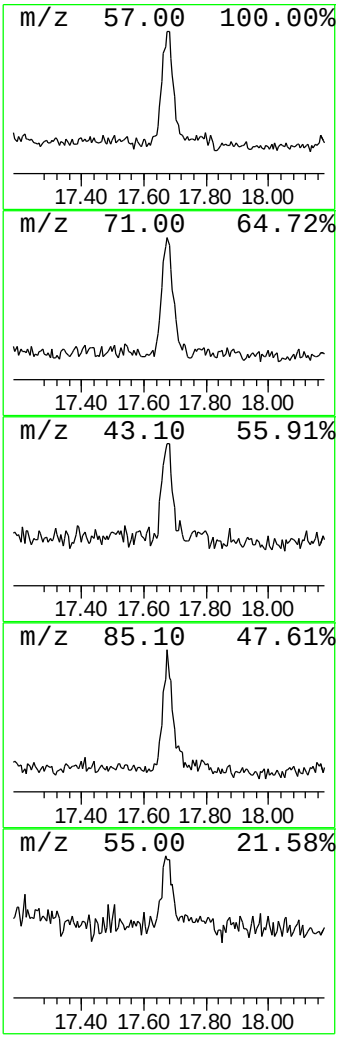
****

Peak Number 12 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.68	2.78 ng	82993	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	86
2	Hexacosane	366	C26H54	000630-01-3	80
3	Hentriacontane	437	C31H64	000630-04-6	80
4	Heptacosane	380	C27H56	000593-49-7	78
5	Pentatriacontane	493	C35H72	000630-07-9	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099542.D
Acq On : 16 Oct 2017 14:12
Operator : SJ/JU
Sample : I5875-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TK2064L-T1-T2-T3

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.61	6.61	15.7	ng	467920	1	6.85	595943	20.0
o-Cymene	6.92	16.8	ng	499837	1	6.85	595943	20.0
D-Limonene	6.95	4.2	ng	124136	1	6.85	595943	20.0
Hexanoic acid, 2-...	7.52	2.4	ng	105676	2	8.13	891315	20.0
Cyclohexanemethan...	7.96	3.3	ng	145452	2	8.13	891315	20.0
Naphthalene, 1-me...	8.94	2.8	ng	122490	2	8.13	891315	20.0
1-Docosene	13.84	2.5	ng	65803	5	14.01	525483	20.0
Eicosane	16.40	2.0	ng	60008	6	15.49	597426	20.0
Hentriacontane	16.98	2.1	ng	62493	6	15.49	597426	20.0
Octacosane	17.68	2.8	ng	82993	6	15.49	597426	20.0