LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117367.D
Acq On : 10 Oct 2019 18:29
Operator : JU
Sample : K5297-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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-BF091319.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	5.004	493	496	509	rBV	39540	61639	5.49%	0.513%
2	5.422	563	567	588	rBV	811940	915901	81.61%	7.623%
3	6.440	736	740	758	rBV	982733	1054348	93.95%	8.775%
4	6.569	758	762	768	rVV	1213466	1055964	94.09%	8.788%
5	6.616	768	770	775	rVB	20491	19414	1.73%	0.162%
6	6.792	797	800	807	rBV	277645	250688	22.34%	2.086%
7	6.951	823	827	830	rBV	827569	761738	67.87%	6.340%
8	7.045	840	843	845	rBV	39994	36121	3.22%	0.301%
9	7.116	850	855	856	rVV2	26402	28233	2.52%	0.235%
10	7.134	856	858	862	rVB2	24763	21975	1.96%	0.183%
11	7.328	887	891	893	rBV	171119	143987	12.83%	1.198%
12	7.357	893	896	906	rVB	651182	657078	58.55%	5.468%
13	7.563	925	931	934	rBV	104065	98594	8.79%	0.821%
14	7.592	934	936	941	rVB	31644	27446	2.45%	0.228%
15	7.681	947	951	956	rBV	24633	27280	2.43%	0.227%
16	7.728	956	959	960	rVV2	17818	18341	1.63%	0.153%
17	7.745	960	962	968	rVV	87808	107213	9.55%	0.892%
18	7.810	970	973	977	rVV2	179597	200933	17.90%	1.672%
19	7.845	977	979	981	rVV	30663	28822	2.57%	0.240%
20	7.892	985	987	989	rVV2	20884	21229	1.89%	0.177%
21	7.945	993	996	999	rVB	28945	24606	2.19%	0.205%
22	8.075	1005	1018	1024	rBV2	349978	572326	51.00%	4.763%
23	8.122	1024	1026	1031	rVV	75686	77829	6.93%	0.648%
24	8.163	1031	1033	1036	rVB	24219	19840	1.77%	0.165%
25	8.351	1062	1065	1072	rVB3	34232	38485	3.43%	0.320%
26	8.463	1080	1084	1087	rBV	43331	43525	3.88%	0.362%
27	8.545	1094	1098	1101	rBV	25633	25356	2.26%	0.211%
28	8.581	1101	1104	1109	rVB5	18683	27072	2.41%	0.225%
29	8.639	1109	1114	1116	rVB2	8608	12749	1.14%	0.106%
30	8.663	1116	1118	1122	rBV2	18742	20417	1.82%	0.170%
31	8.792	1137	1140	1148	rBV	81158	85090	7.58%	0.708%
32	8.886	1151	1156	1166	rVB	59411	76703	6.83%	0.638%
33	9.151	1197	1201	1214	rBV	1231360	1122284	100.00%	9.340%
34	9.545	1265	1268	1274	rVB	95175	89717	7.99%	0.747%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117367.D
Acq On : 10 Oct 2019 18:29
Operator : JU
Sample : K5297-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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-BF091319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.828	1312	1316	1319	rBV	419777	381244	33.97%	3.173%
36	9.863	1319	1322	1332	rVB	106236	111344	9.92%	0.927%
37	10.039	1349	1352	1356	rBV	47259	44707	3.98%	0.372%
38	10.380	1407	1410	1416	rBV2	76108	76965	6.86%	0.641%
39	10.622	1447	1451	1464	rBV	661166	676715	60.30%	5.632%
40	11.216	1547	1552	1555	rVB	16071	17299	1.54%	0.144%
41	11.316	1565	1569	1571	rBV	389896	353985	31.54%	2.946%
42	11.339	1571	1573	1579	rVV	267376	260776	23.24%	2.170%
43	11.398	1579	1583	1587	rVB	22626	31392	2.80%	0.261%
44	11.563	1607	1611	1616	rVB2	11119	13063	1.16%	0.109%
45	11.822	1653	1655	1656	rBV	15485	12588	1.12%	0.105%
46	11.845	1656	1659	1665	rVB4	31703	50681	4.52%	0.422%
47	11.933	1671	1674	1677	rBV	36681	37949	3.38%	0.316%
48	12.533	1772	1776	1779	rBV	152006	142406	12.69%	1.185%
49	12.563	1779	1781	1786	rVB	50947	42648	3.80%	0.355%
50	12.763	1809	1815	1822	rBV	97403	117864	10.50%	0.981%
51	12.898	1834	1838	1841	rBV	1055721	875432	78.00%	7.286%
52	13.033	1859	1861	1865	rBV	14211	14247	1.27%	0.119%
53	13.792	1983	1990	2006	rBV6	37653	98161	8.75%	0.817%
54	13.927	2009	2013	2015	rVV	18883	18020	1.61%	0.150%
55	13.963	2015	2019	2028	rVB	243746	279026	24.86%	2.322%
56	14.110	2040	2044	2046	rBV3	12290	15562	1.39%	0.130%
57	14.410	2092	2095	2098	rBV	22058	21173	1.89%	0.176%
58	14.504	2109	2111	2115	rBV5	7016	12222	1.09%	0.102%
59	14.710	2141	2146	2151	rBV2	36506	43270	3.86%	0.360%
60	15.039	2198	2202	2205	rVB2	37175	42014	3.74%	0.350%
61	15.410	2260	2265	2278	rVB	217067	328530	29.27%	2.734%
62	15.821	2331	2335	2340	rVB2	33878	42953	3.83%	0.357%
63	16.062	2374	2376	2383	rVB8	8737	12663	1.13%	0.105%
64	16.310	2414	2418	2422	rVB5	16503	26820	2.39%	0.223%
65	16.486	2445	2448	2455	rVB9	9197	16583	1.48%	0.138%
66	16.862	2507	2512	2513	rBV5	10663	12786	1.14%	0.106%
67	17.033	2539	2541	2547	rVB7	6431	11702	1.04%	0.097%

Sum of corrected areas: 12015733

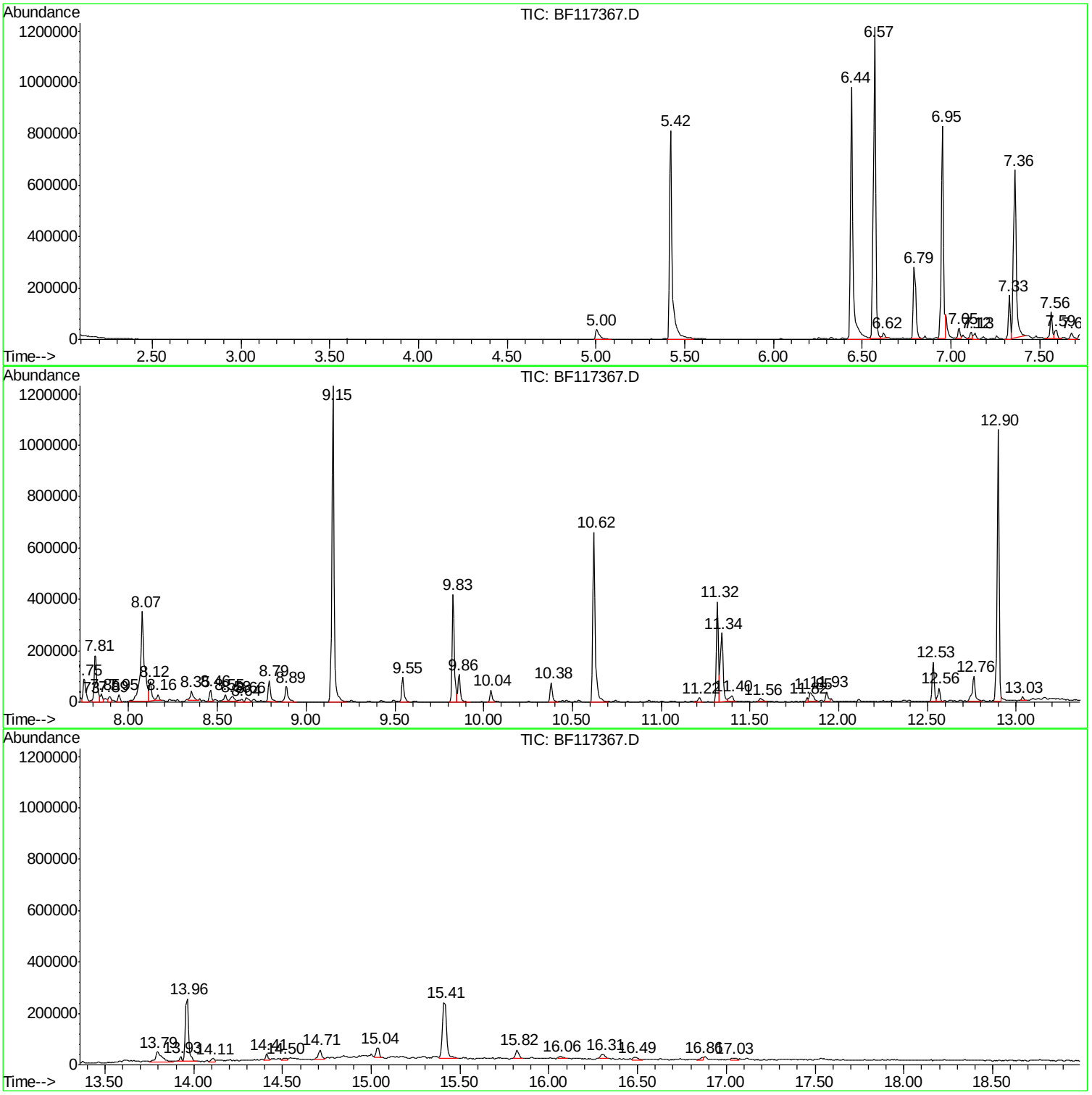
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117367.D
Acq On : 10 Oct 2019 18:29
Operator : JU
Sample : K5297-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117367.D
Acq On : 10 Oct 2019 18:29
Operator : JU
Sample : K5297-04
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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

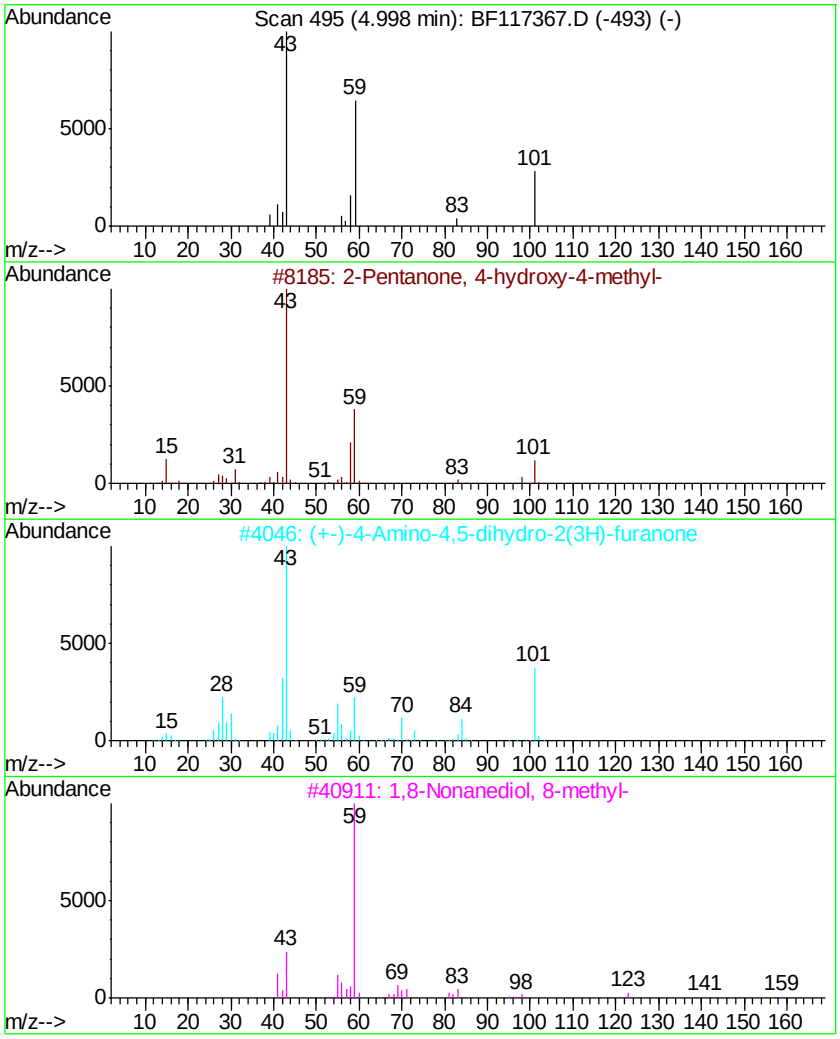
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

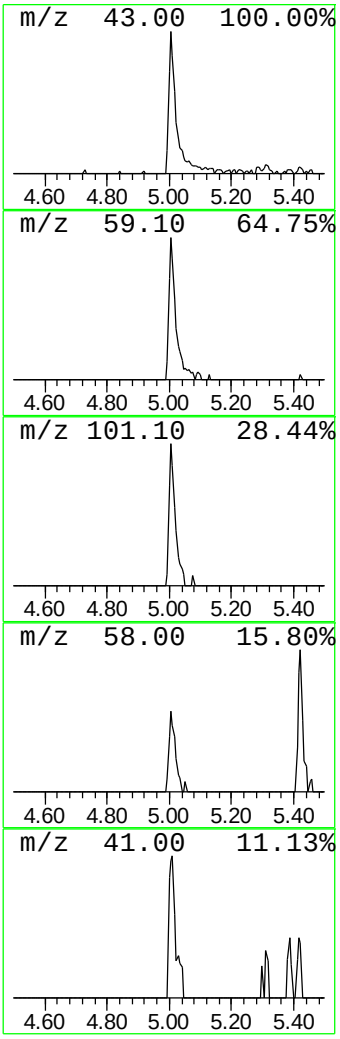
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.92 ng	61639	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	28
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117367.D
Acq On : 10 Oct 2019 18:29
Operator : JU
Sample : K5297-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

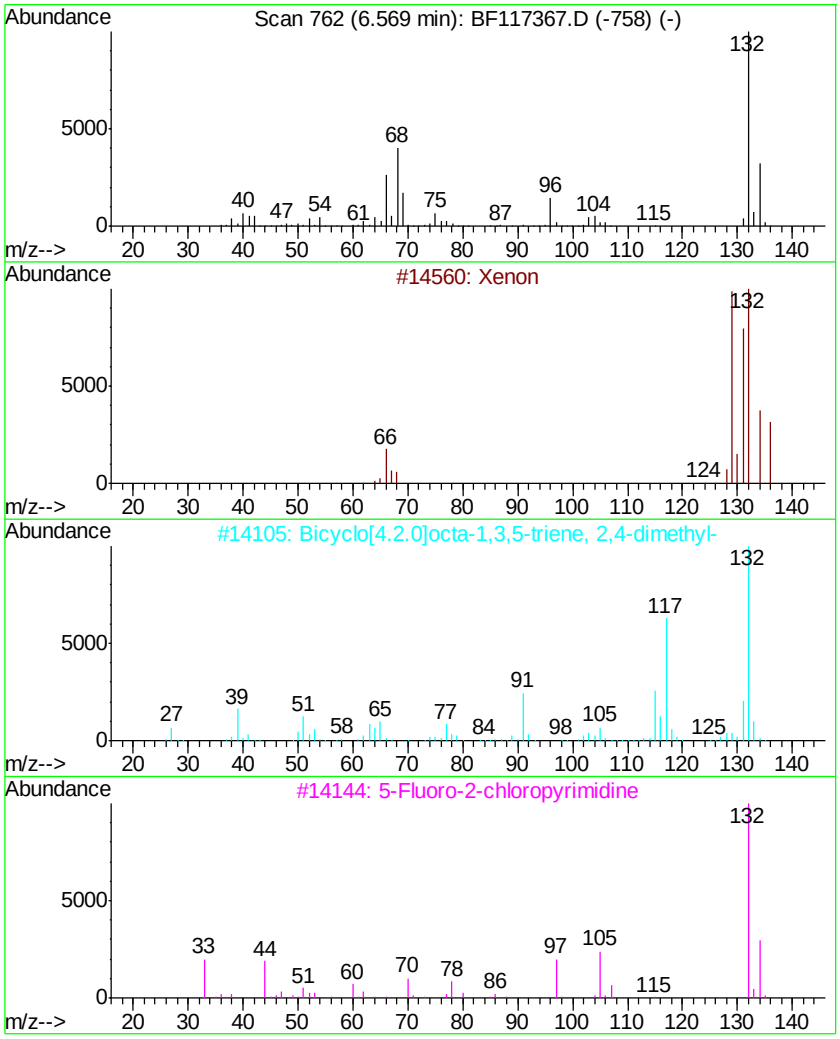
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

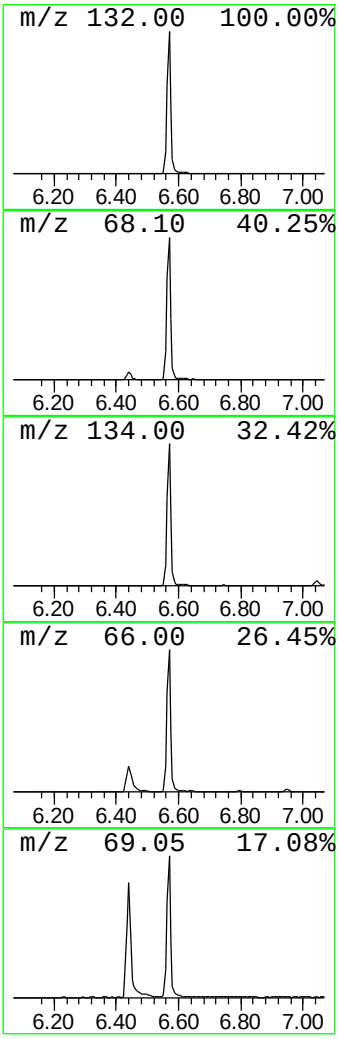
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	84.25 ng	1055960	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Xenon	132	Xe	007440-63-3	9
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117367.D
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Operator : JU
Sample : K5297-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

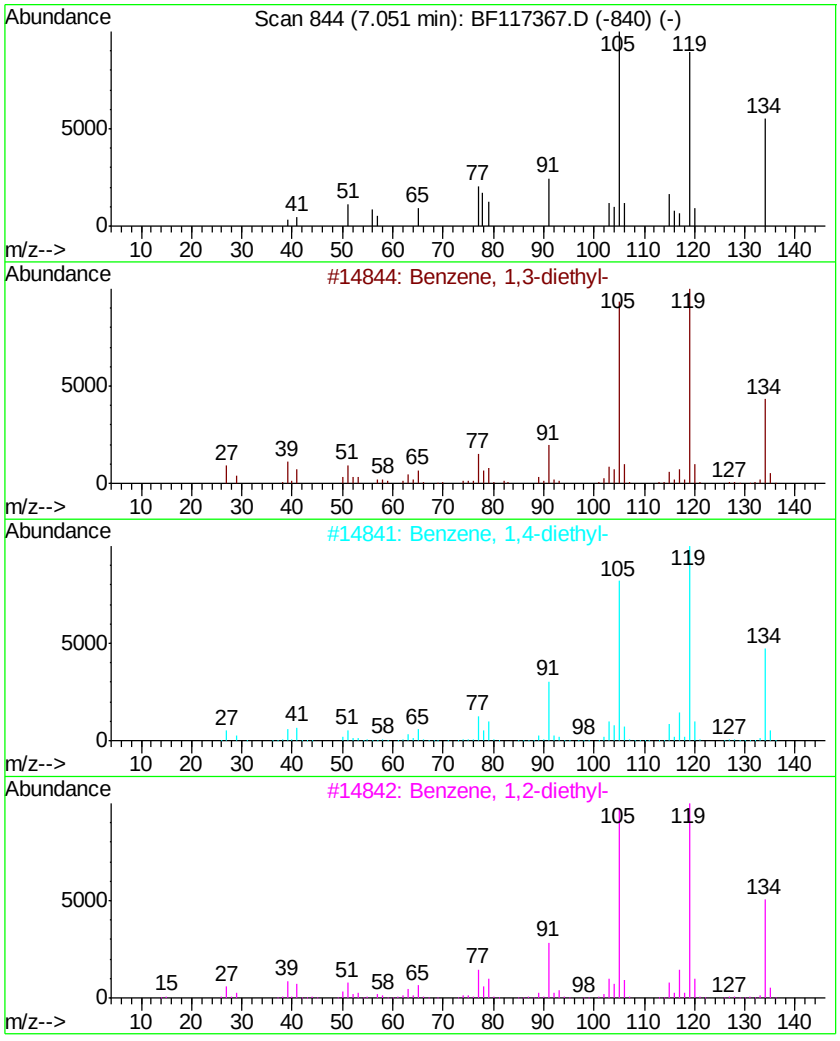
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

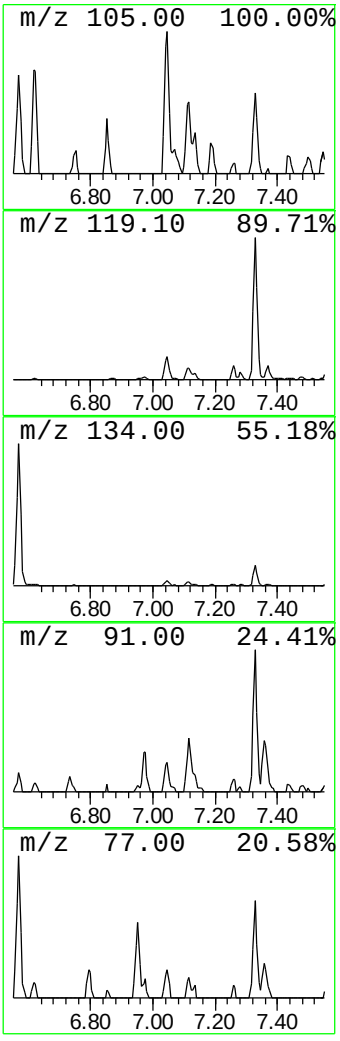
****

Peak Number 4 Benzene, 1,3-diethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	2.88 ng	36121	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	94
2	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	94
3	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	94
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117367.D
Acq On : 10 Oct 2019 18:29
Operator : JU
Sample : K5297-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

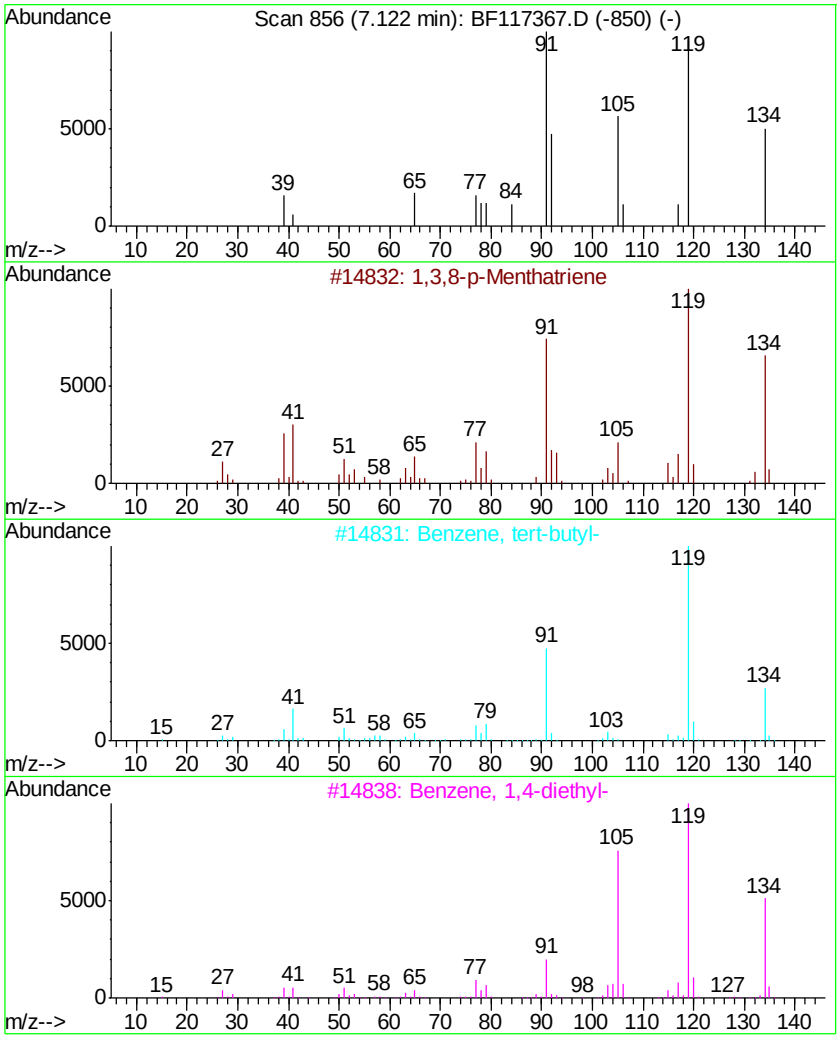
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

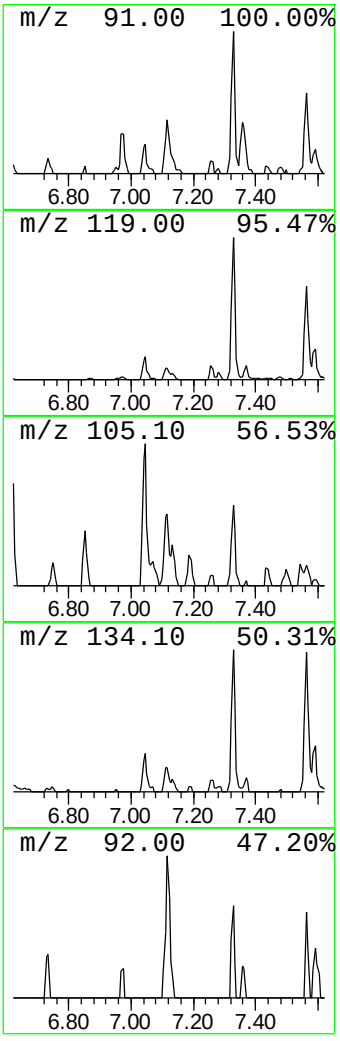
****

Peak Number 5 1,3,8-p-Menthatriene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	2.25 ng	28233	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,8-p-Menthatriene	134	C10H14	018368-95-1	81
2	Benzene, tert-butyl-	134	C10H14	000098-06-6	72
3	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	70
4	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	70
5	Benzofuran, 2,3-dihydro-2-methyl-	134	C9H10O	001746-11-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117367.D
Acq On : 10 Oct 2019 18:29
Operator : JU
Sample : K5297-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

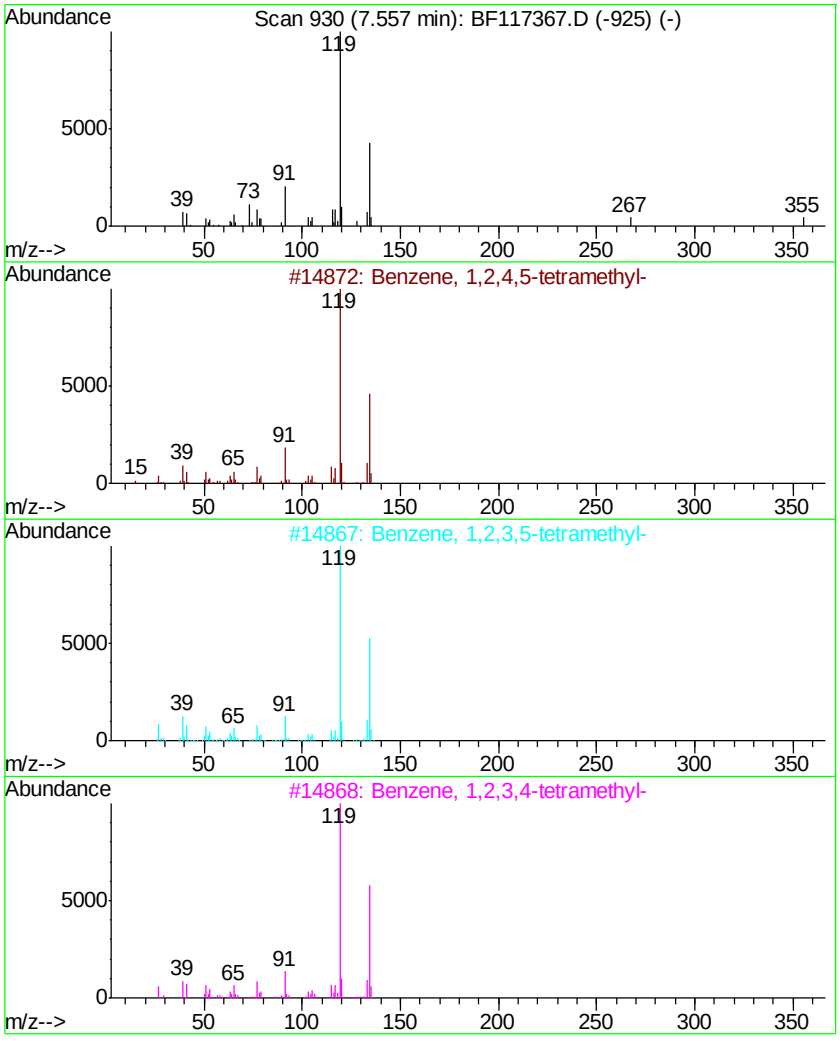
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

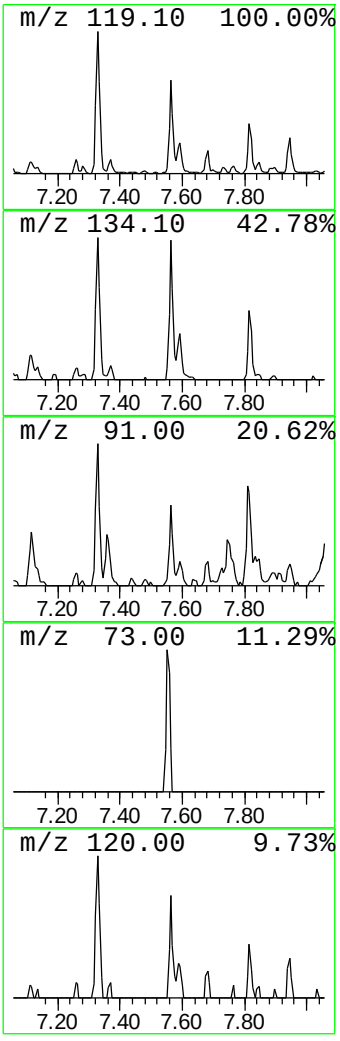
****

Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	3.45 ng	98594	Naphthalene-d8	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117367.D
Acq On : 10 Oct 2019 18:29
Operator : JU
Sample : K5297-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

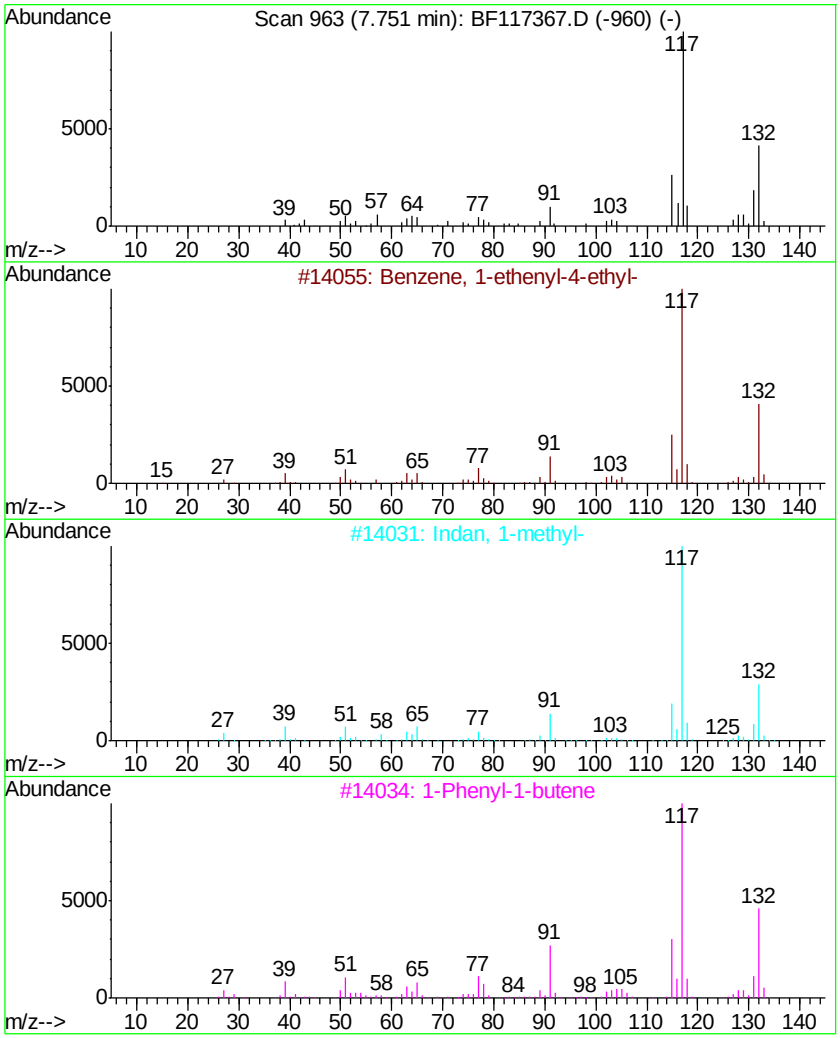
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

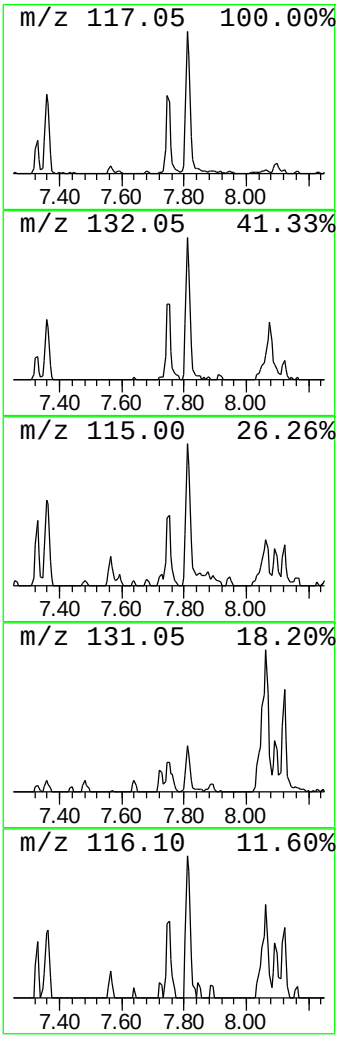
****

Peak Number 7 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	3.75 ng	107213	Naphthalene-d8	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
2	Indan, 1-methyl-	132	C10H12	000767-58-8	90
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	86
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117367.D
Acq On : 10 Oct 2019 18:29
Operator : JU
Sample : K5297-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

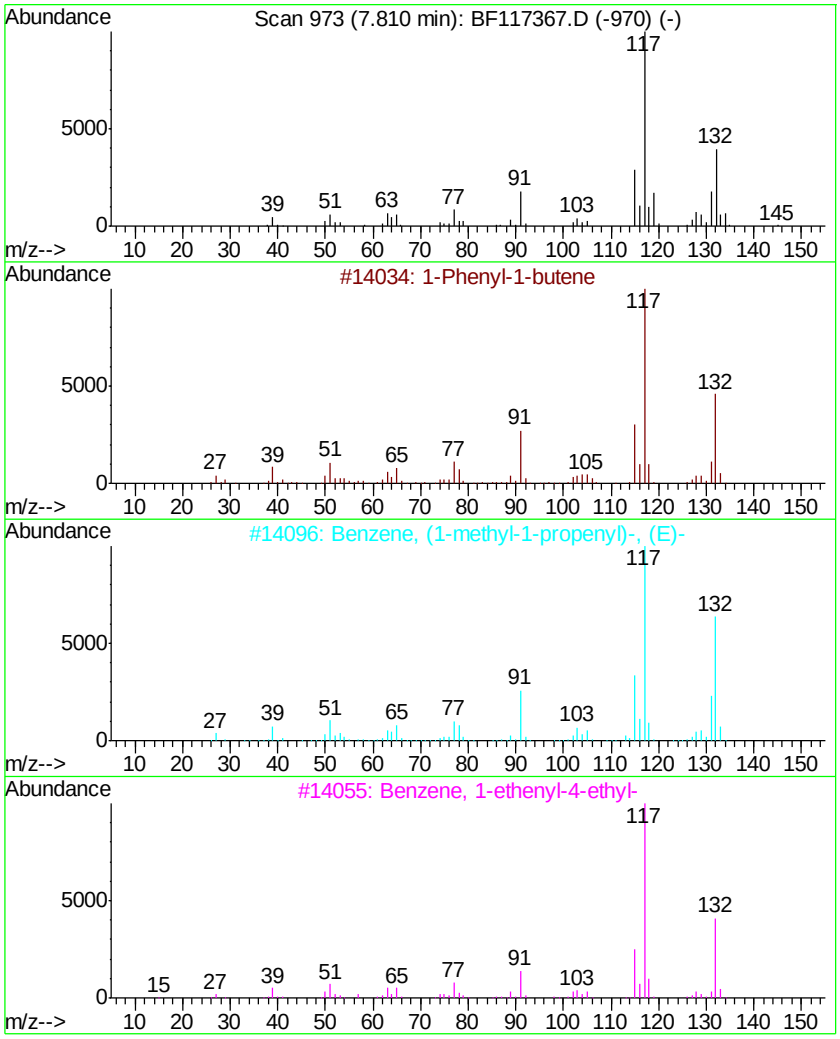
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

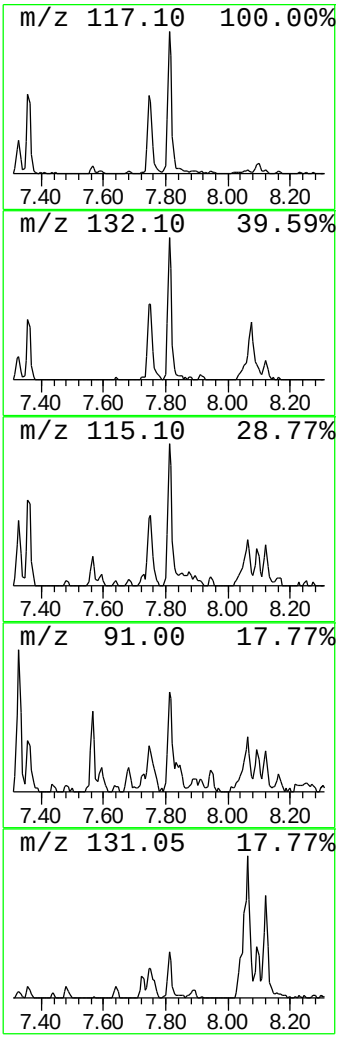
****

Peak Number 8 1-Phenyl-1-butene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	7.02 ng	200933	Naphthalene-d8	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	93
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	92
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	91
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	90
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117367.D
Acq On : 10 Oct 2019 18:29
Operator : JU
Sample : K5297-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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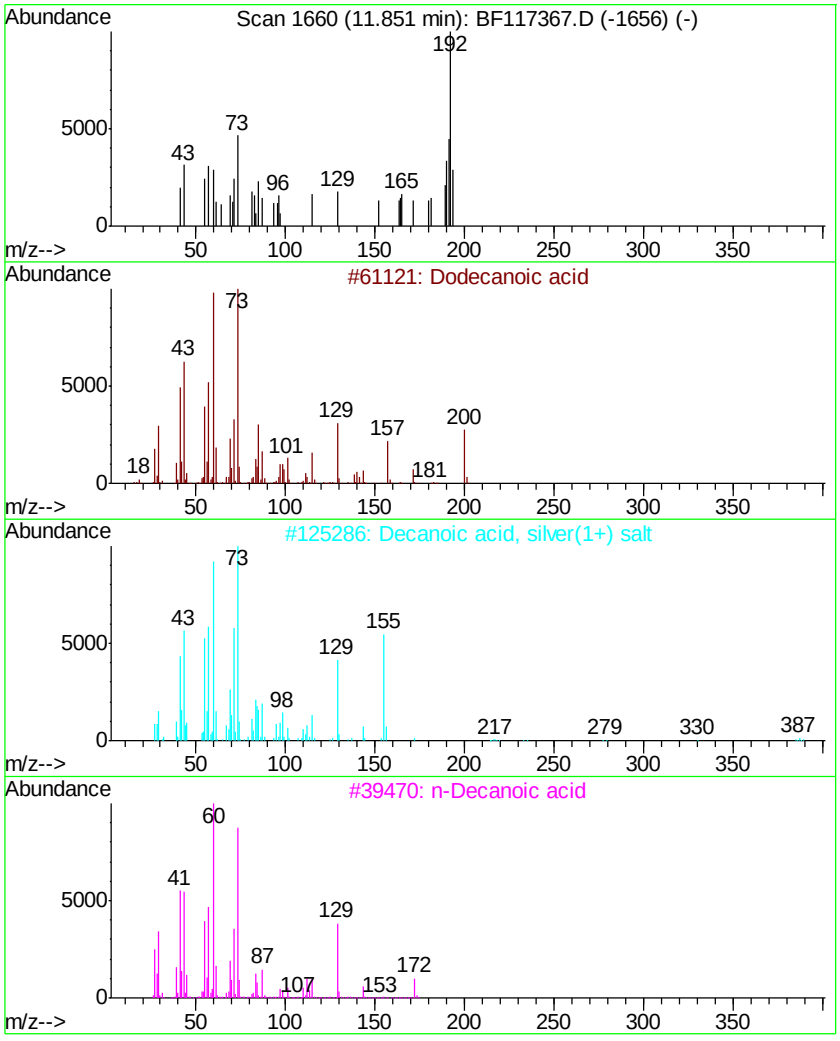
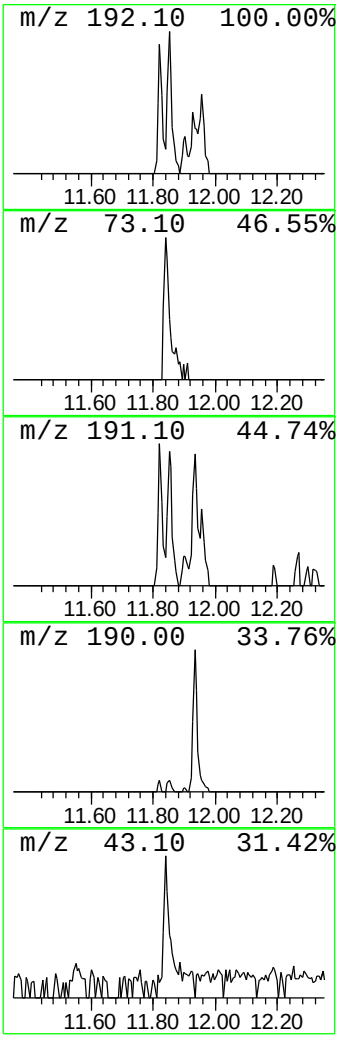
Peak Number 9 Dodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.86 ng	50681	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	53
2	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	38
5	Nonanoic acid	158	C9H18O2	000112-05-0	35





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Sample : K5297-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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TIC Integration Parameters: LSCINT.P

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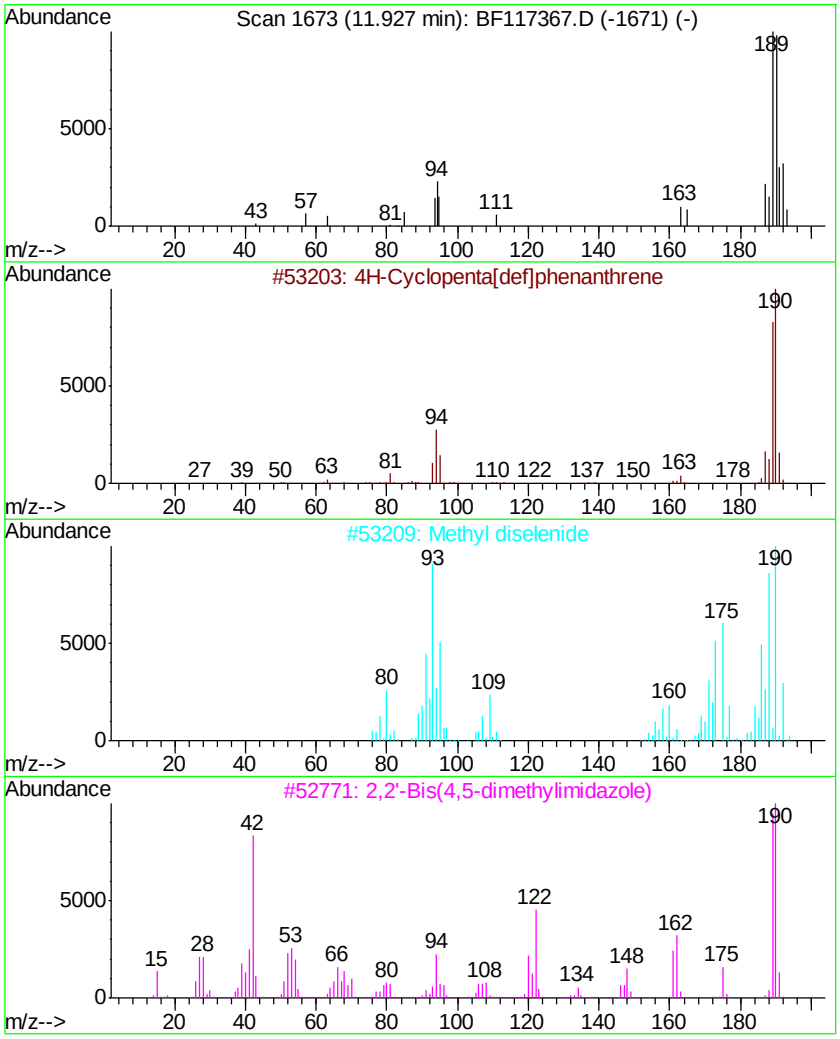
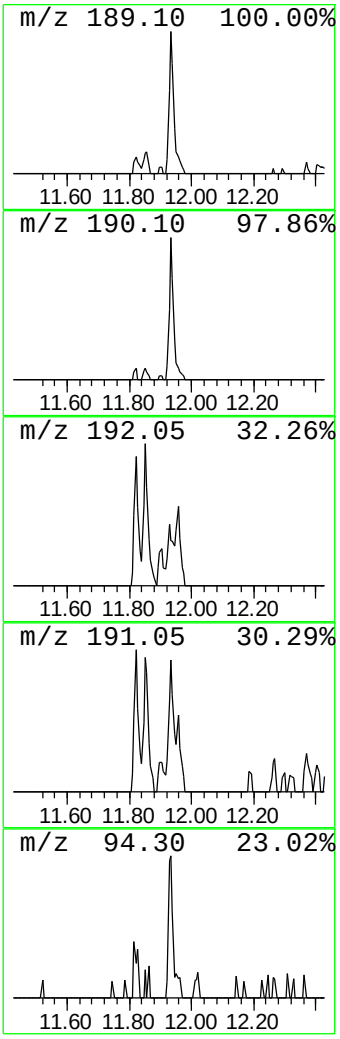
Peak Number 10 4H-Cyclopenta[def]phenanthrene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.14 ng	37949	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	Methyl diselenide	190	C2H6Se2	007101-31-7	55
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
4	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	42
5	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	40





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Instrument : BNA_F
ClientSampleId : TP-1

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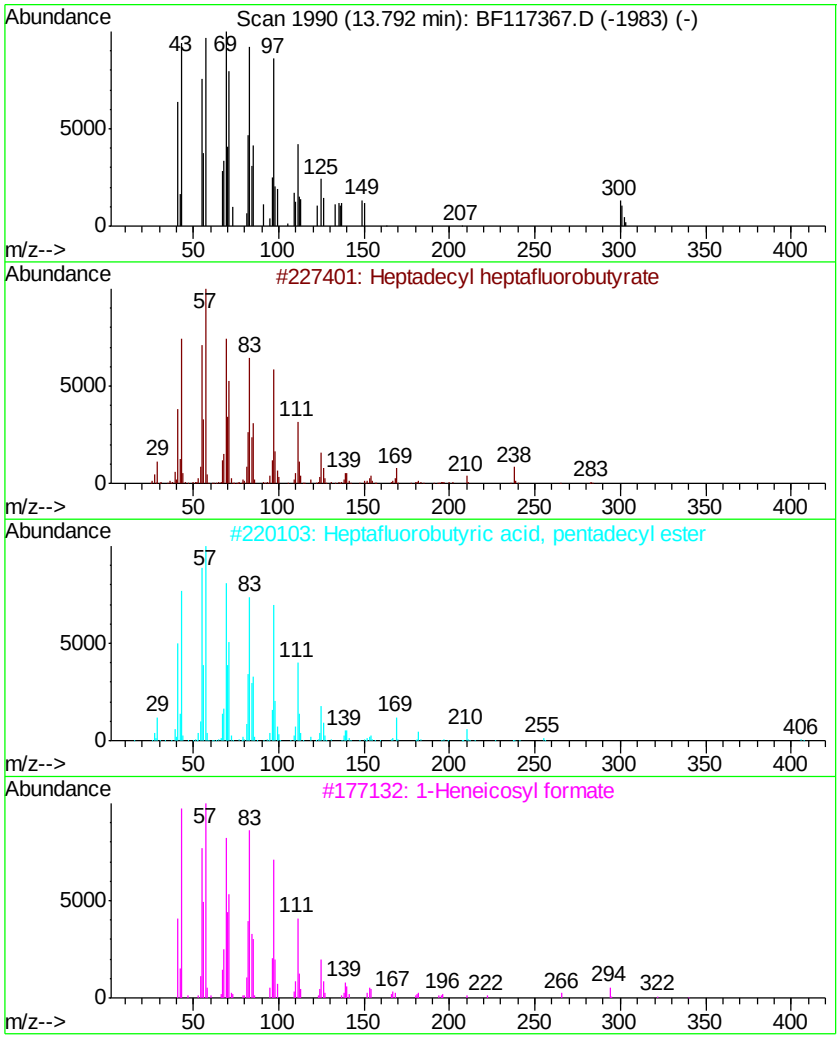
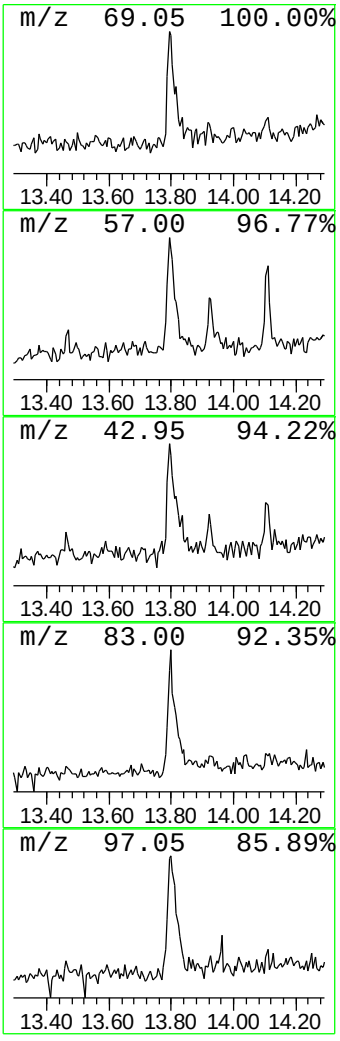
Peak Number 11 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	7.04 ng	98161	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	81
4	1-Heptacosanol	396	C27H56O	002004-39-9	81
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	76





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ALS Vial : 9 Sample Multiplier: 1

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ClientSampleId : TP-1

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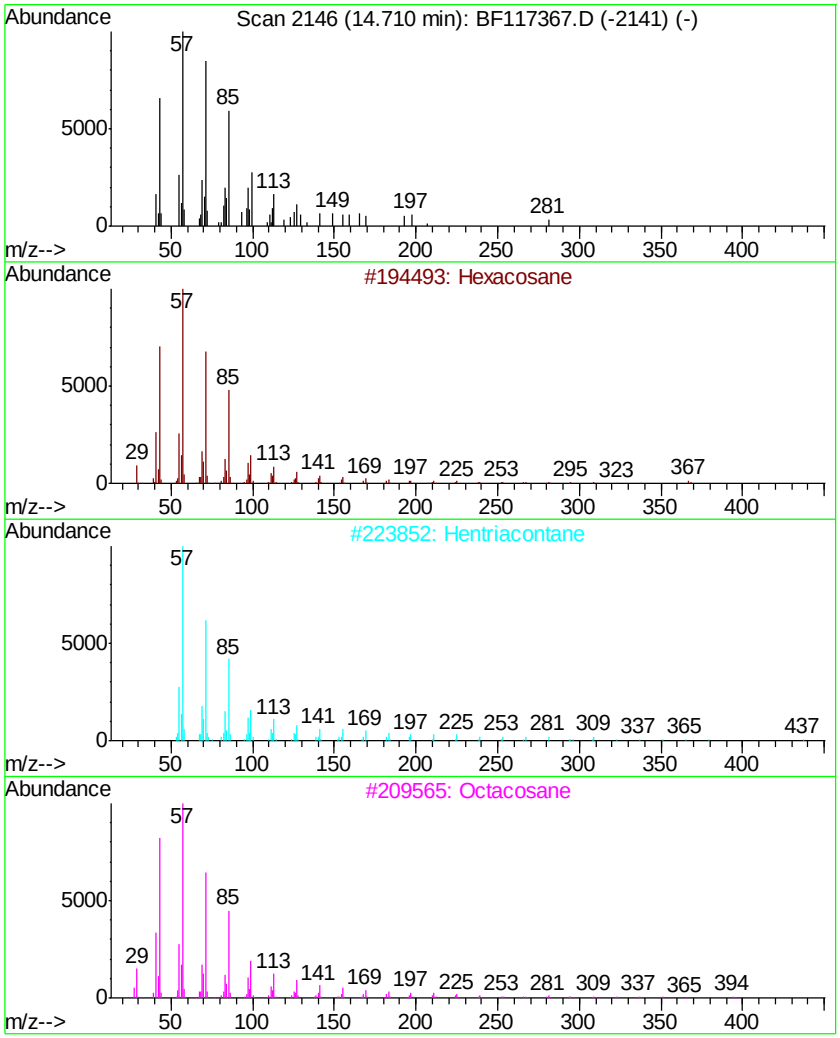
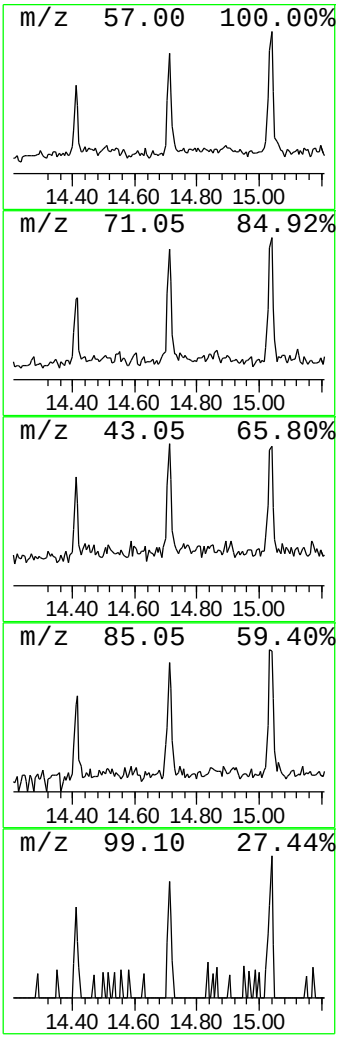
Peak Number 12 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.63 ng	43270	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Hentriacontane	437	C31H64	000630-04-6	83
3	Octacosane	394	C28H58	000630-02-4	80
4	Heneicosane	296	C21H44	000629-94-7	80
5	Heptacosane	380	C27H56	000593-49-7	72





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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

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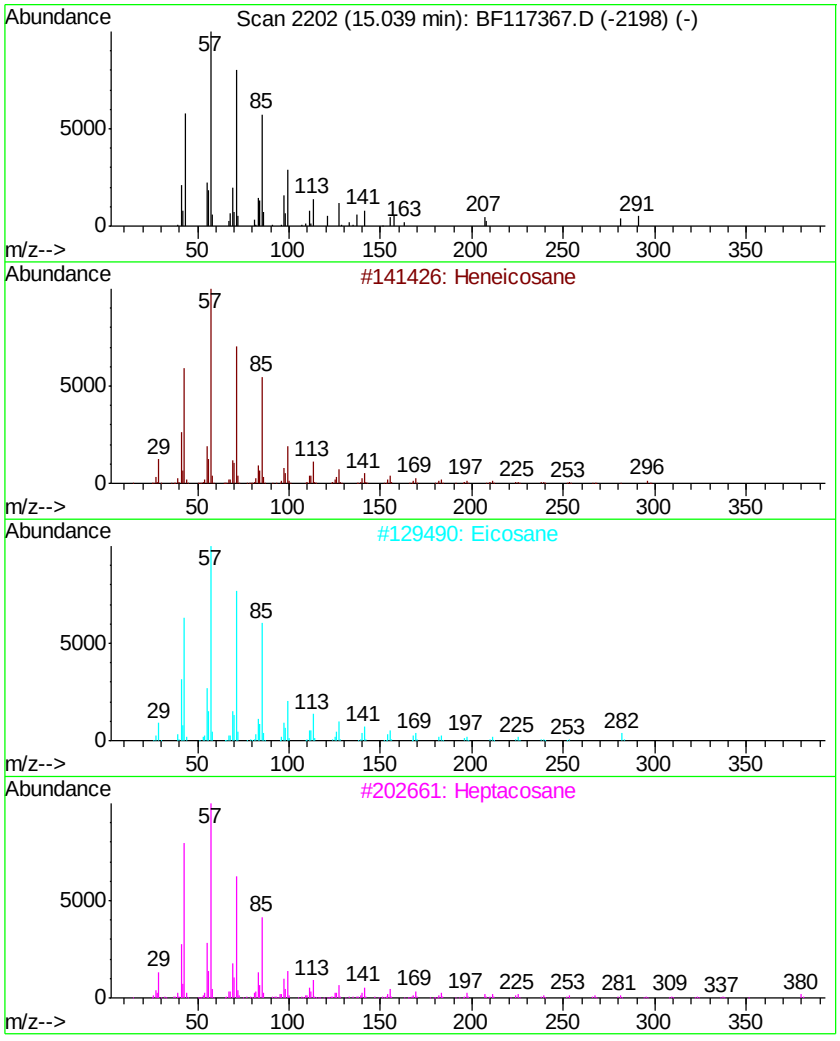
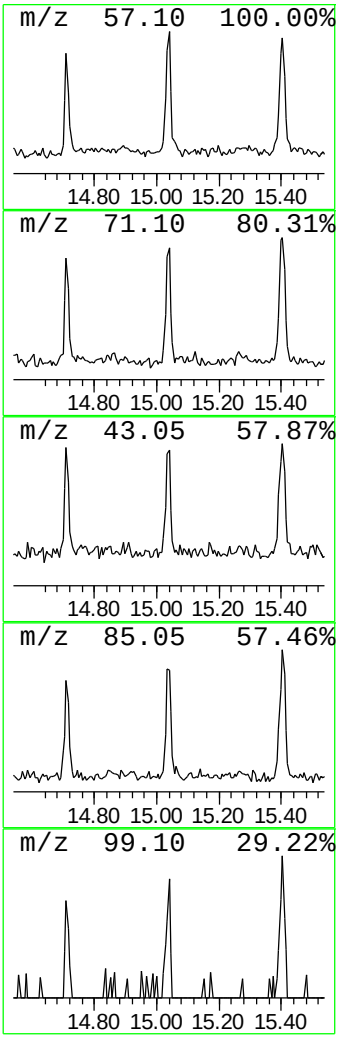
Peak Number 13 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	2.56 ng	42014	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Eicosane	282	C20H42	000112-95-8	90
3	Heptacosane	380	C27H56	000593-49-7	86
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Hentriacontane	437	C31H64	000630-04-6	86





Tentatively Identified Compound (LSC) summary

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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...	5.00	4.9	ng	61639	1	6.79	250688	20.0
unknown6.57	6.57	84.3	ng	1055960	1	6.79	250688	20.0
Benzene, 1,3-diet...	7.05	2.9	ng	36121	1	6.79	250688	20.0
1,3,8-p-Menthatriene	7.12	2.3	ng	28233	1	6.79	250688	20.0
Benzene, 1,2,4,5-...	7.56	3.5	ng	98594	2	8.07	572326	20.0
Benzene, 1-etheny...	7.75	3.8	ng	107213	2	8.07	572326	20.0
1-Phenyl-1-butene	7.81	7.0	ng	200933	2	8.07	572326	20.0
Dodecanoic acid	11.85	2.9	ng	50681	4	11.32	353985	20.0
4H-Cyclopenta[def...	11.93	2.1	ng	37949	4	11.32	353985	20.0
Heptadecyl heptaf...	13.79	7.0	ng	98161	5	13.96	279026	20.0
Hexacosane	14.71	2.6	ng	43270	6	15.42	328530	20.0
Heneicosane	15.04	2.6	ng	42014	6	15.42	328530	20.0