LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121319\
Data File : BF118194.D
Acq On : 13 Dec 2019 18:59
Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

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-BF120619.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	2.116	3	5	11	rVB	298938	333788	6.68%	1.058%
2	5.075	503	508	520	rVB	342339	411180	8.23%	1.303%
3	5.487	574	578	586	rBV	2098851	1959198	39.22%	6.210%
4	6.498	745	750	762	rBV	2266824	2136956	42.78%	6.773%
5	6.640	769	774	777	rBV	2659646	2298915	46.02%	7.286%
6	6.869	809	813	818	rBV	730852	641475	12.84%	2.033%
7	7.022	835	839	843	rBV	2259986	1945341	38.94%	6.166%
8	7.428	904	908	919	rBV	1364793	1379322	27.61%	4.372%
9	8.151	1024	1031	1039	rBV	881052	821955	16.45%	2.605%
10	9.228	1210	1214	1218	rBV	3001624	2807605	56.20%	8.899%
11	9.316	1223	1229	1231	rBV4	148002	238865	4.78%	0.757%
12	9.545	1265	1268	1271	rBV3	272516	360127	7.21%	1.141%
13	9.586	1273	1275	1279	rVB3	168009	192791	3.86%	0.611%
14	9.634	1279	1283	1286	rBV2	951528	1216080	24.34%	3.854%
15	9.786	1305	1309	1311	rBV4	452309	666626	13.34%	2.113%
16	9.822	1312	1315	1318	rVV3	596133	802228	16.06%	2.543%
17	9.863	1319	1322	1324	rBV3	429799	569634	11.40%	1.805%
18	9.916	1328	1331	1335	rVB	1160538	1388124	27.79%	4.400%
19	10.181	1373	1376	1379	rBV2	1188745	1310109	26.23%	4.152%
20	10.239	1384	1386	1387	rBV	678972	588341	11.78%	1.865%
21	10.592	1443	1446	1450	rVB	2820658	3147469	63.01%	9.976%
22	10.869	1490	1493	1499	rVB	4312057	4995554	100.00%	15.833%
23	15.174	2222	2225	2230	rVB	229560	253424	5.07%	0.803%
24	15.557	2286	2290	2297	rVB2	655272	921638	18.45%	2.921%
25	16.010	2363	2367	2372	rVB2	113923	164504	3.29%	0.521%

Sum of corrected areas: 31551249

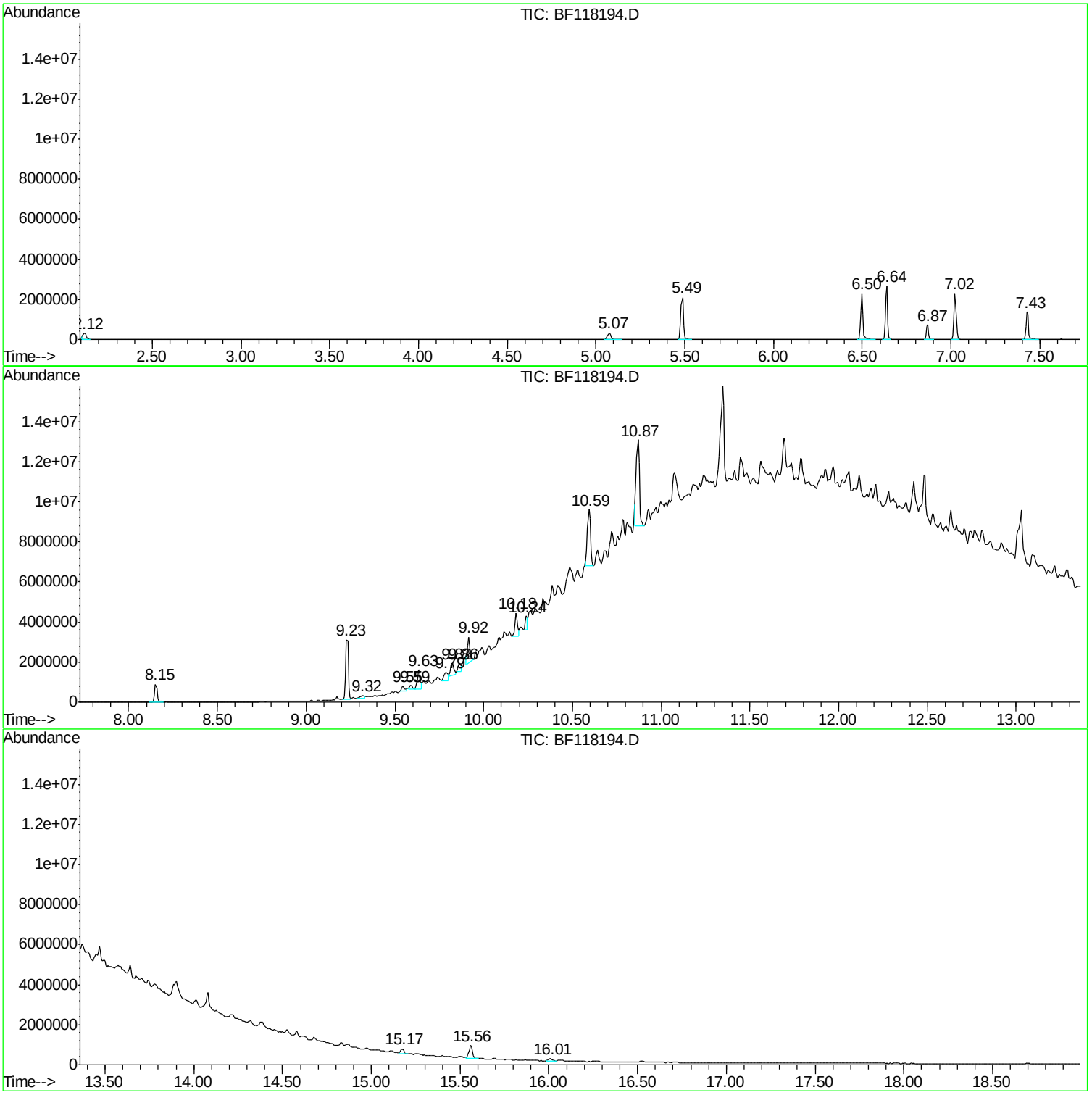
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121319\
Data File : BF118194.D
Acq On : 13 Dec 2019 18:59
Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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Data File : BF118194.D
Acq On : 13 Dec 2019 18:59
Operator : JU
Sample : K6274-01
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ClientSampleId : T2-COMP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

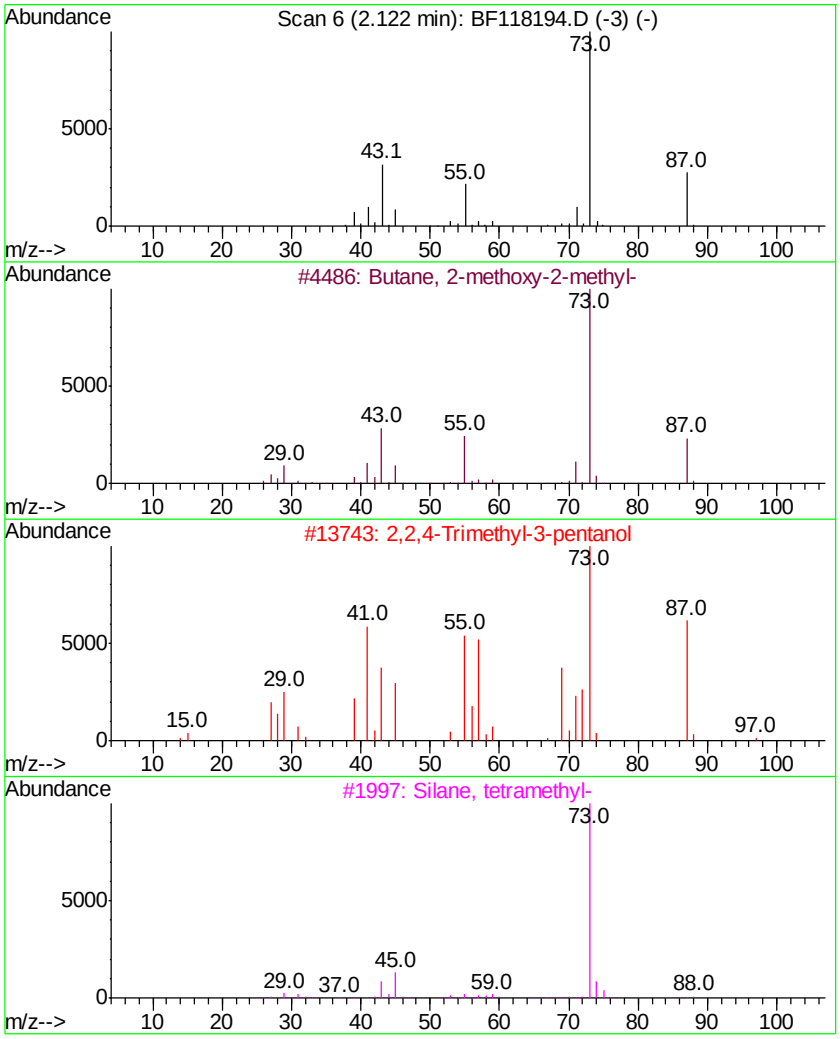
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

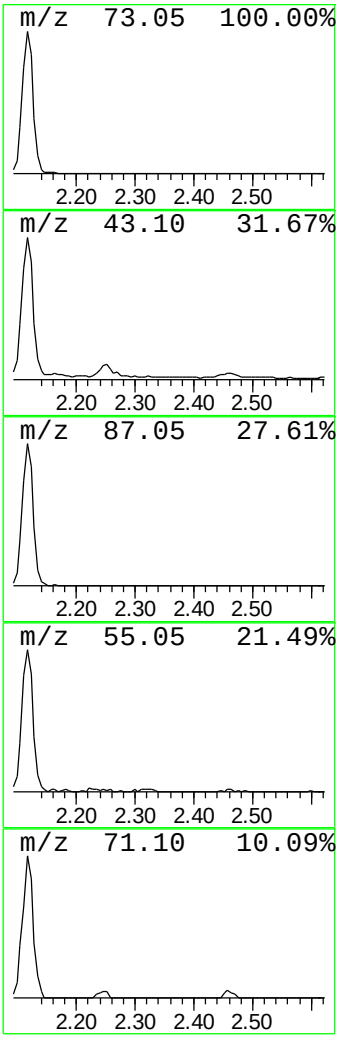
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	10.41 ng	333788	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

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Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

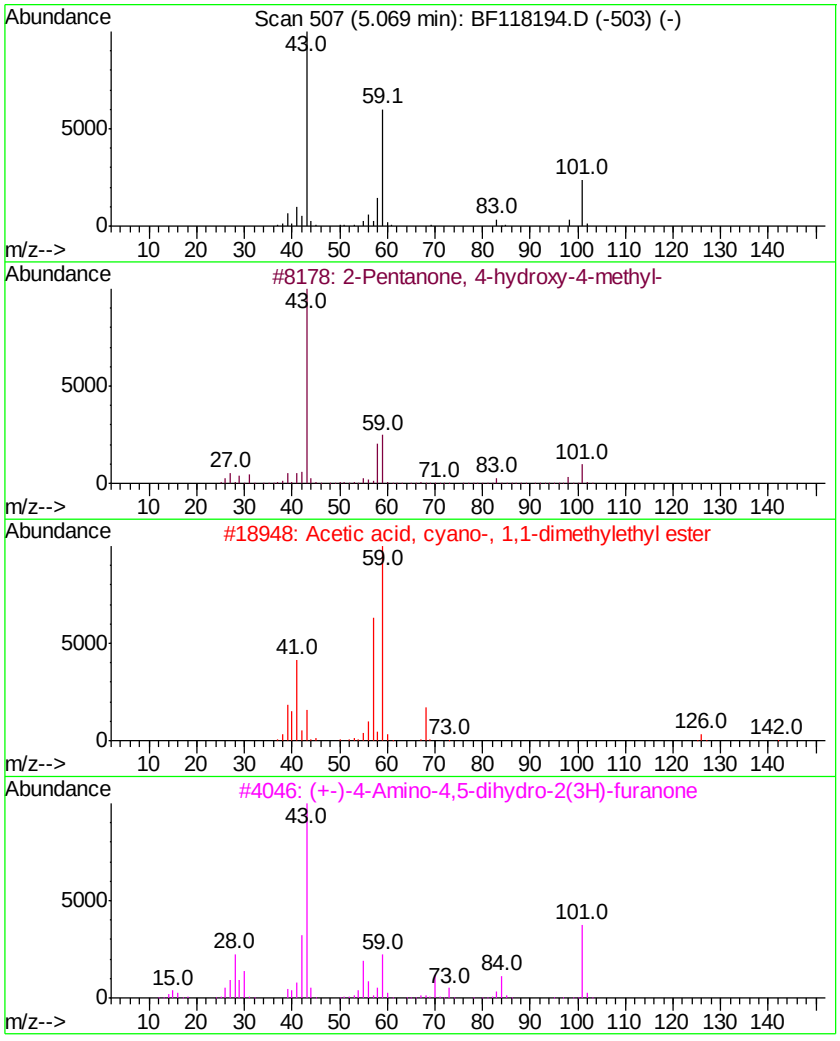
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

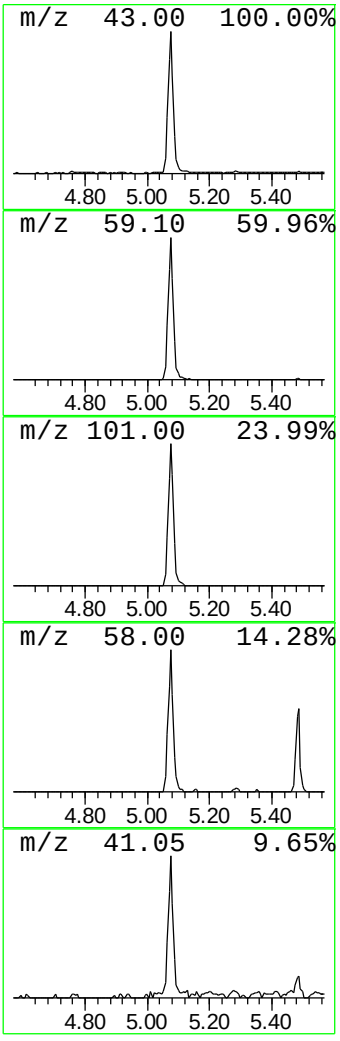
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	12.82 ng	411180	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Butane	58	C4H10	000106-97-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Data File : BF118194.D
Acq On : 13 Dec 2019 18:59
Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

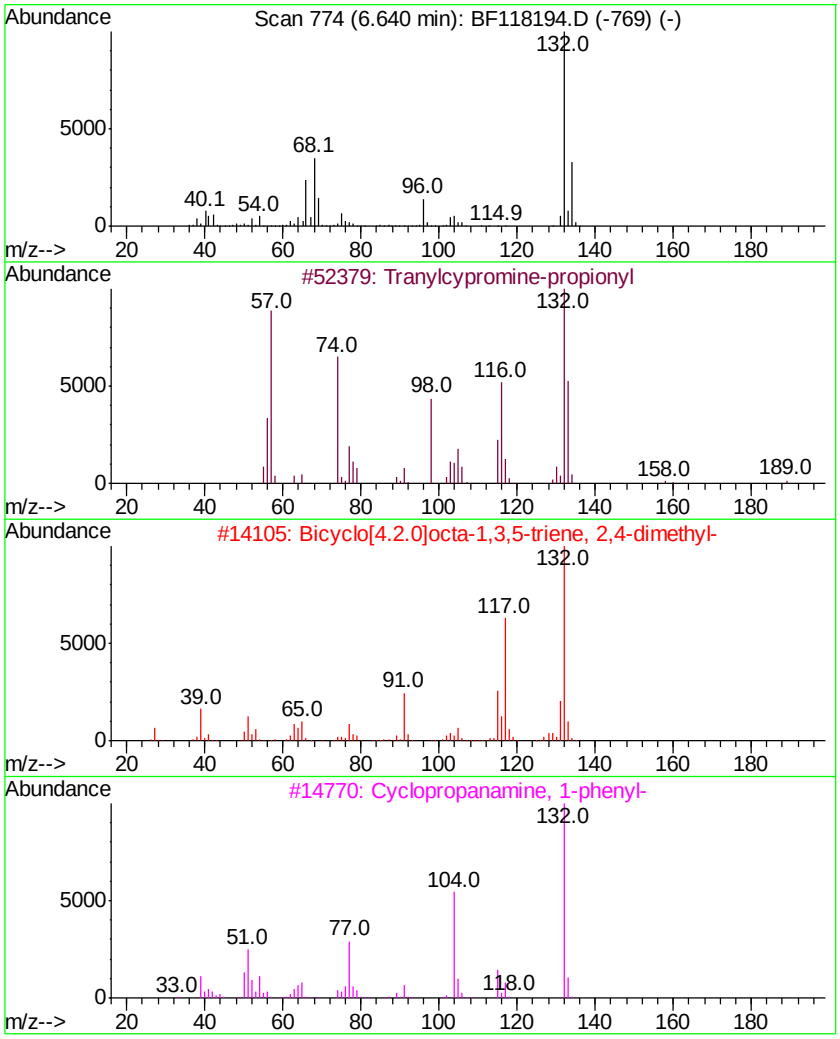
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

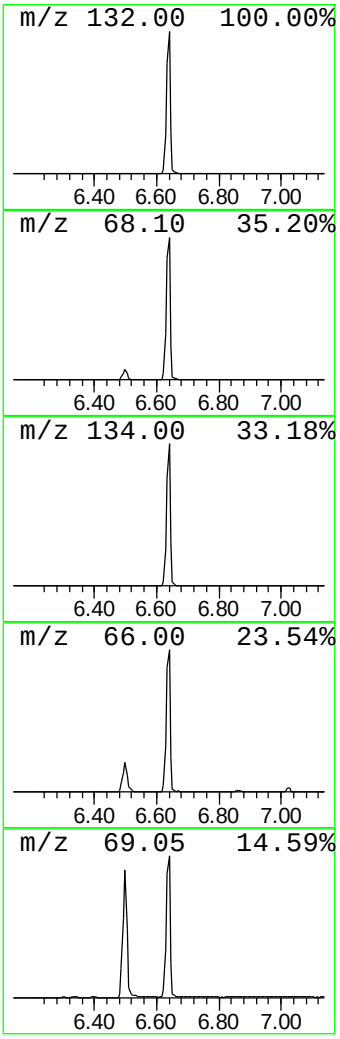
****

Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	71.68 ng	2298920	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

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Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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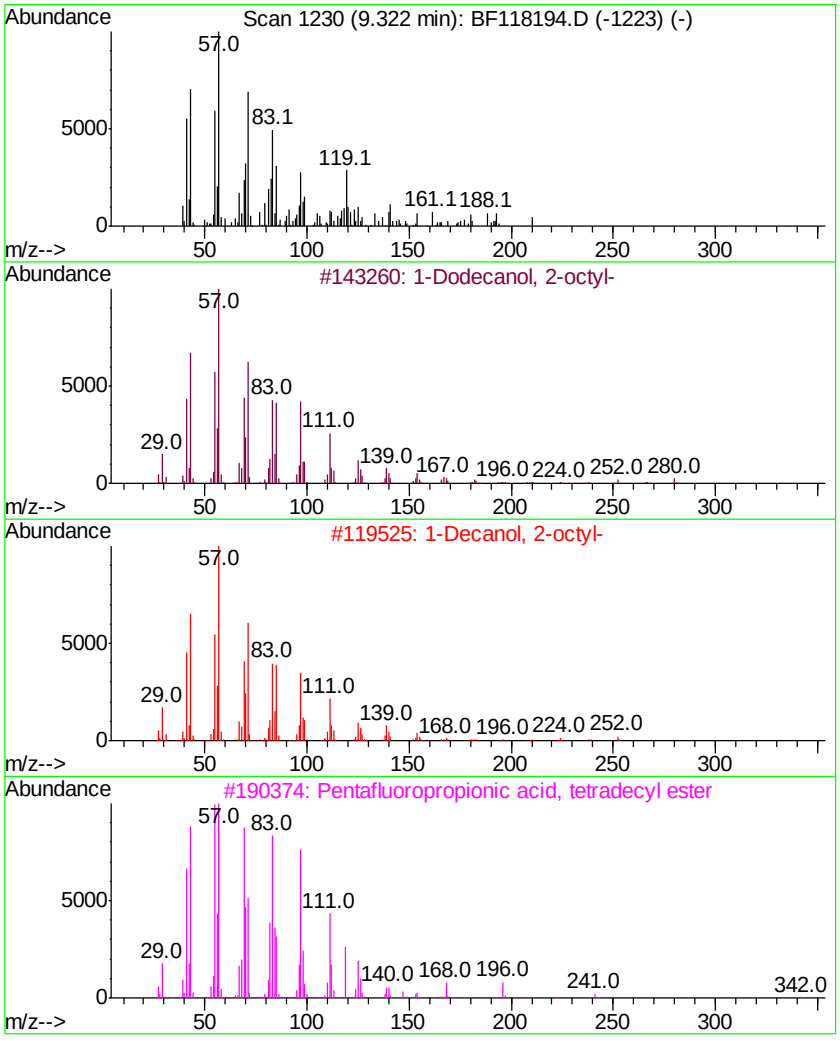
TIC Integration Parameters: LSCINT.P

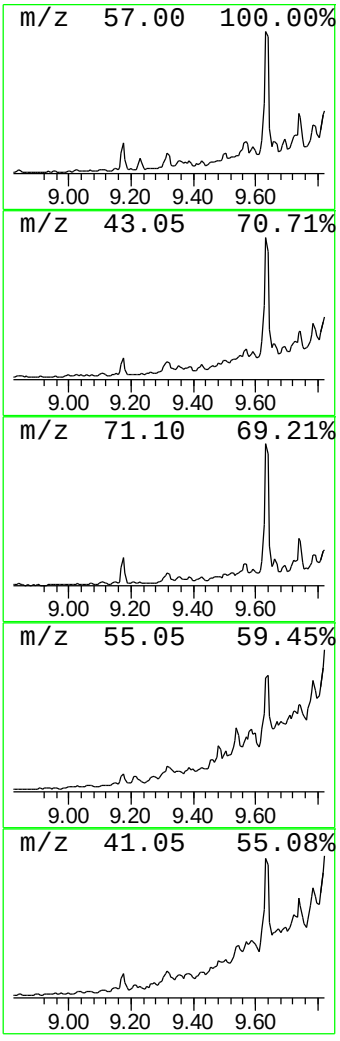
****

Peak Number 5 1-Dodecanol, 2-octyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.32	3.44 ng	238865	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	52
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	52
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	46
4	1-Eicosanol	298	C20H42O	000629-96-9	43
5	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121319\
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Acq On : 13 Dec 2019 18:59
Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

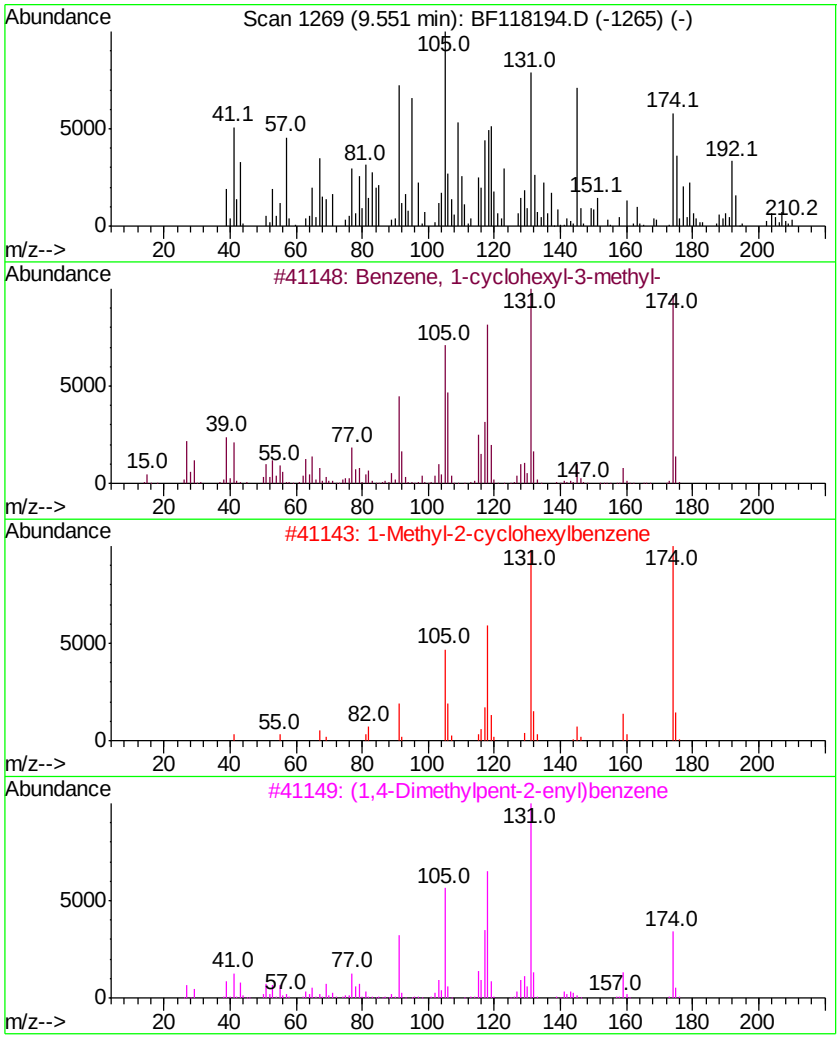
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

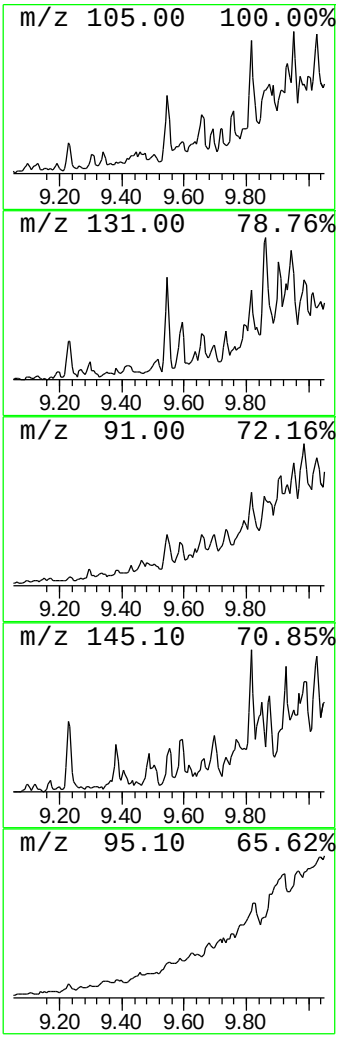
****

Peak Number 6 Benzene, 1-cyclohexyl-3-met... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	5.19 ng	360127	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	89
2	1-Methyl-2-cyclohexylbenzene	174	C13H18	004501-35-3	76
3	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	70
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	38
5	.beta.-Benzal-n-butyramide	175	C11H13NO	007236-47-7	38





Library Search Compound Report

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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
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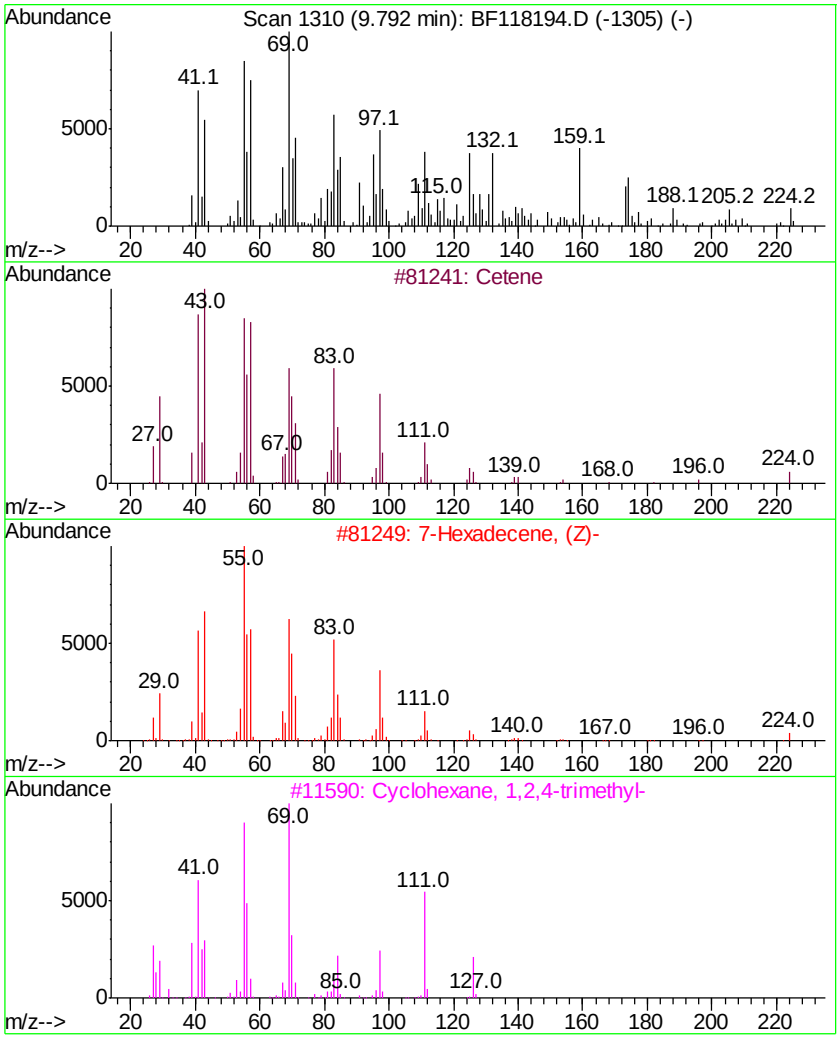
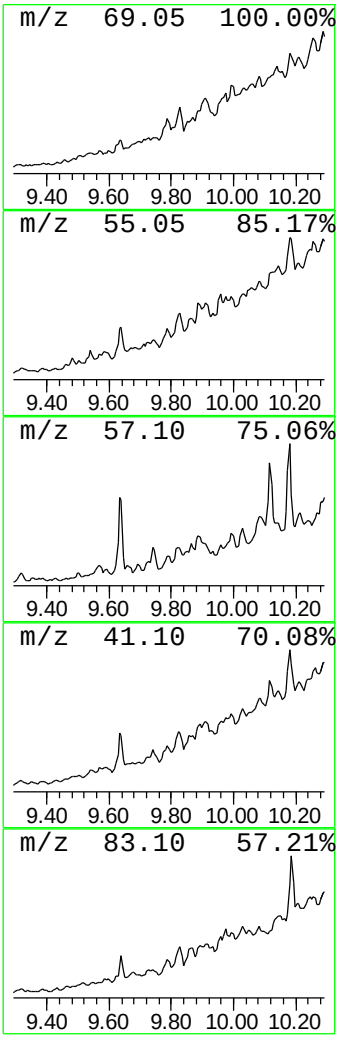
****

Peak Number 7 Cetene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.79	9.60 ng	666626	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	70
2	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	70
3	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	64
4	Trichloroacetic acid, 4-hexadecy...	386	C18H33Cl3O2	1000282-92-4	53
5	Cyclobutanone, 2-(1,1-dimethylet...	126	C8H14O	004579-31-1	50





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TIC Library : C:\DATABASE\NIST11.L
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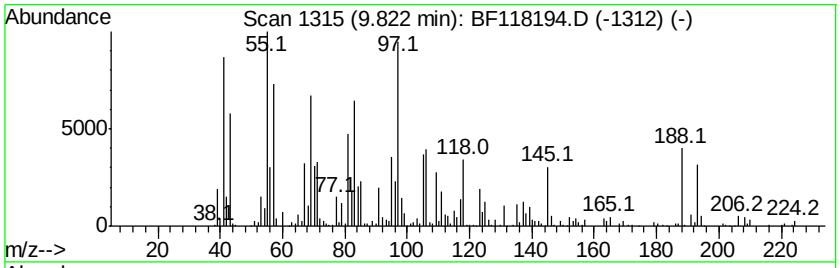
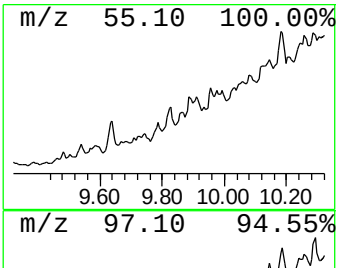
****

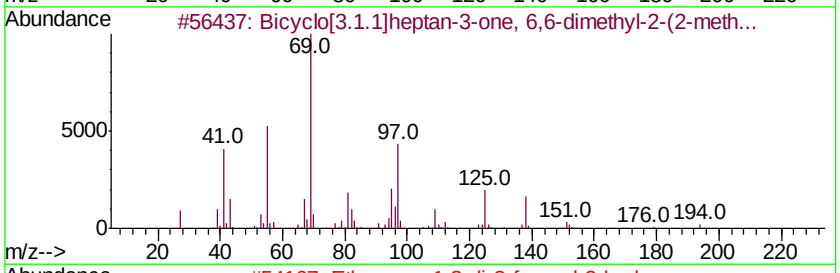
Peak Number 8 unknown9.82 Concentration Rank 7

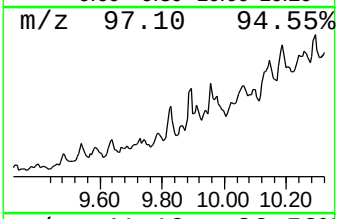
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	11.56 ng	802228	Acenaphthene-d10	9.92

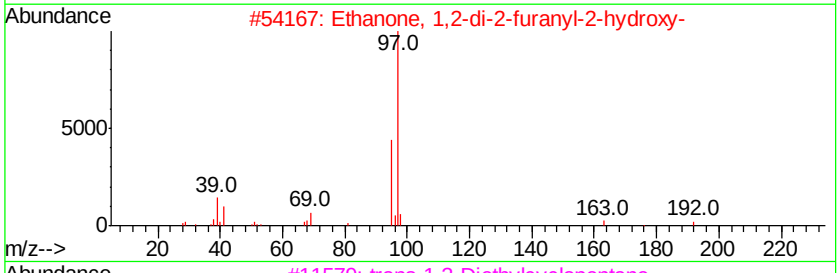
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-3-one, 6,6-...	194	C13H22O	1000163-97-9	38
2	Ethanone, 1,2-di-2-furanyl-2-hyd...	192	C10H8O4	000552-86-3	22
3	trans-1,3-Diethylcyclopentane	126	C9H18	1000113-87-1	20
4	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	18
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	14

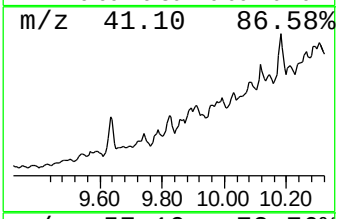


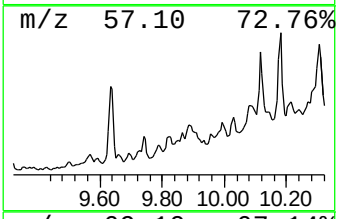


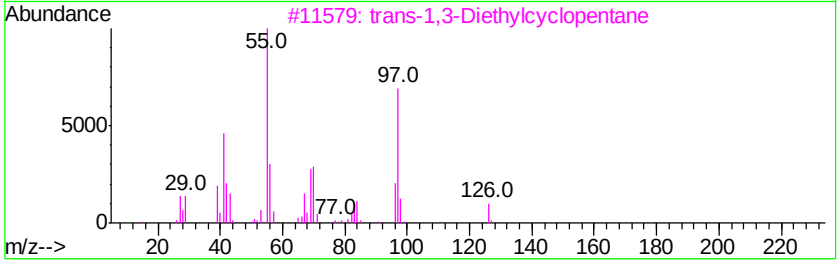


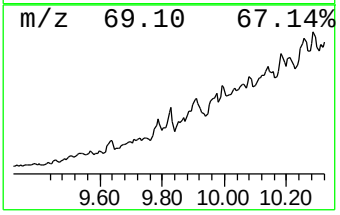












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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
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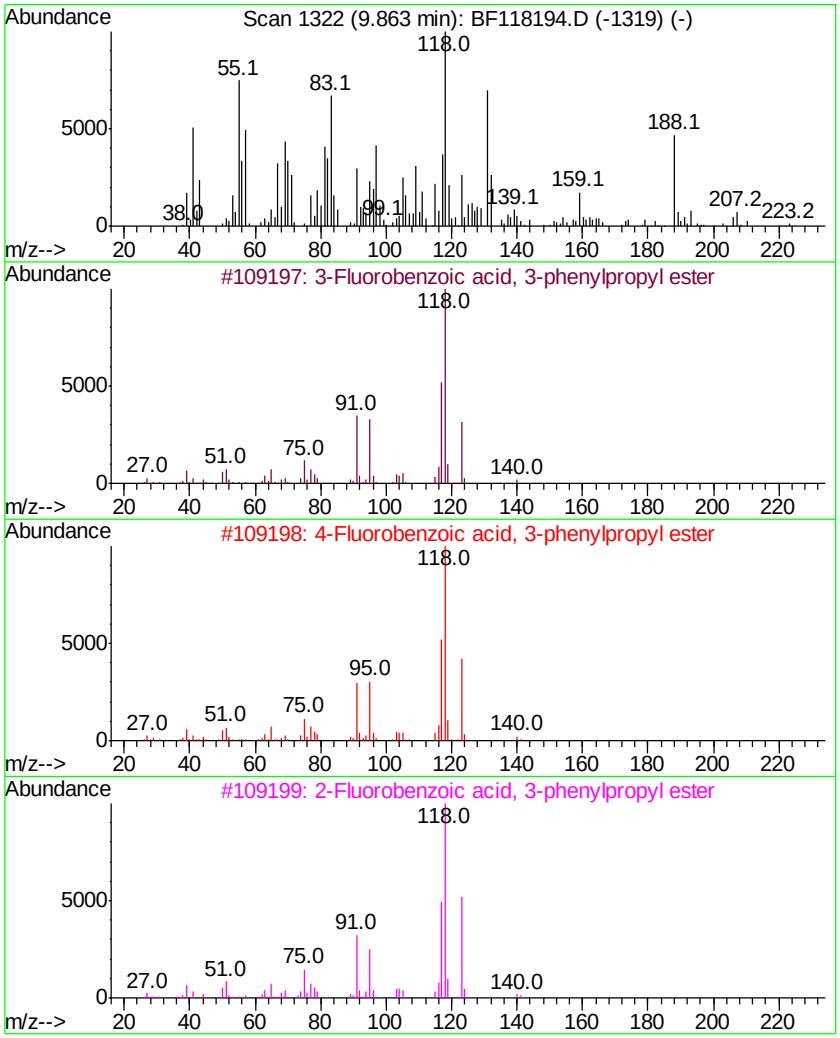
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

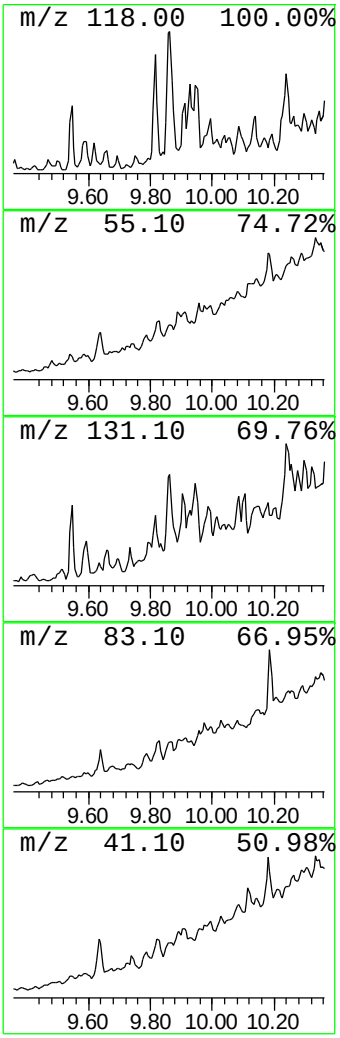
****

Peak Number 9 unknown9.86 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	8.21 ng	569634	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Fluorobenzoic acid, 3-phenylpr...	258	C16H15FO2	1000279-05-0	30
2	4-Fluorobenzoic acid, 3-phenylpr...	258	C16H15FO2	090172-20-6	30
3	2-Fluorobenzoic acid, 3-phenylpr...	258	C16H15FO2	1000278-98-4	27
4	5-Bromopentanoic acid, 3-phenylp...	298	C14H19BrO2	1000293-55-7	22
5	Methyl dichlorophosphate	148	CH3Cl2O2P	000677-24-7	22





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Data File : BF118194.D
Acq On : 13 Dec 2019 18:59
Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

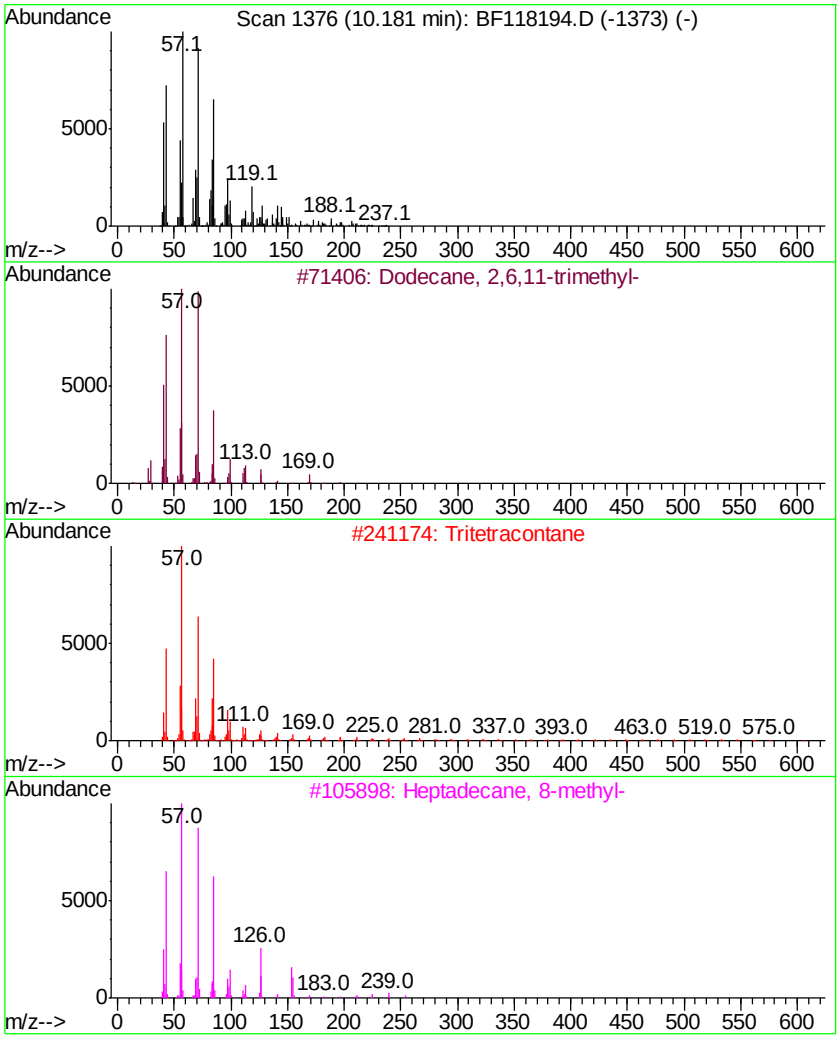
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

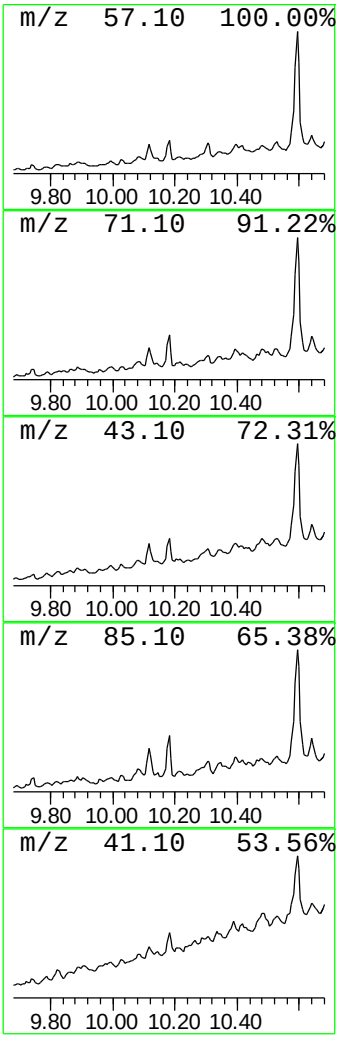
****

Peak Number 10 Dodecane, 2,6,11-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	18.88 ng	1310110	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	70
2	Tritetracontane	605	C43H88	007098-21-7	64
3	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	58
4	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	58
5	Nonadecane	268	C19H40	000629-92-5	52





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Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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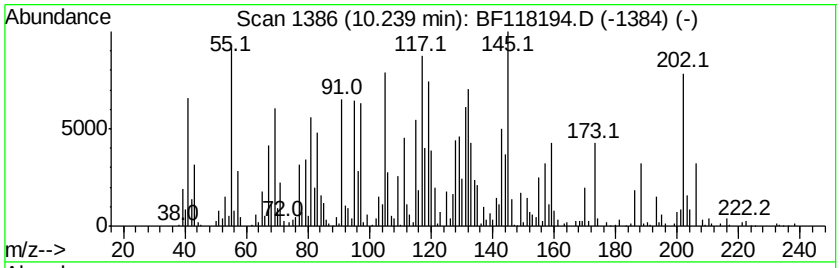
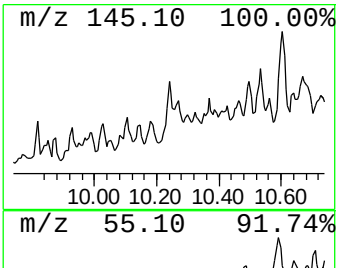
Peak Number 11 Aromadendrene, dehydro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.24	8.48 ng	588341	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aromadendrene, dehydro-	202	C15H22	1000156-12-5	53
2	Benzene, 1-methyl-4-(1,2,2-trime...	202	C15H22	016982-00-6	38
3	Benzene, 1-(1,5-dimethyl-4-hexen...	202	C15H22	000644-30-4	35
4	Cinnamaldehyde, .alpha.-pentyl-	202	C14H18O	000122-40-7	27
5	1H-Indene, 5-hexyl-2,3-dihydro-	202	C15H22	054889-55-3	25





Library Search Compound Report

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Data File : BF118194.D
Acq On : 13 Dec 2019 18:59
Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
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TIC Integration Parameters: LSCINT.P

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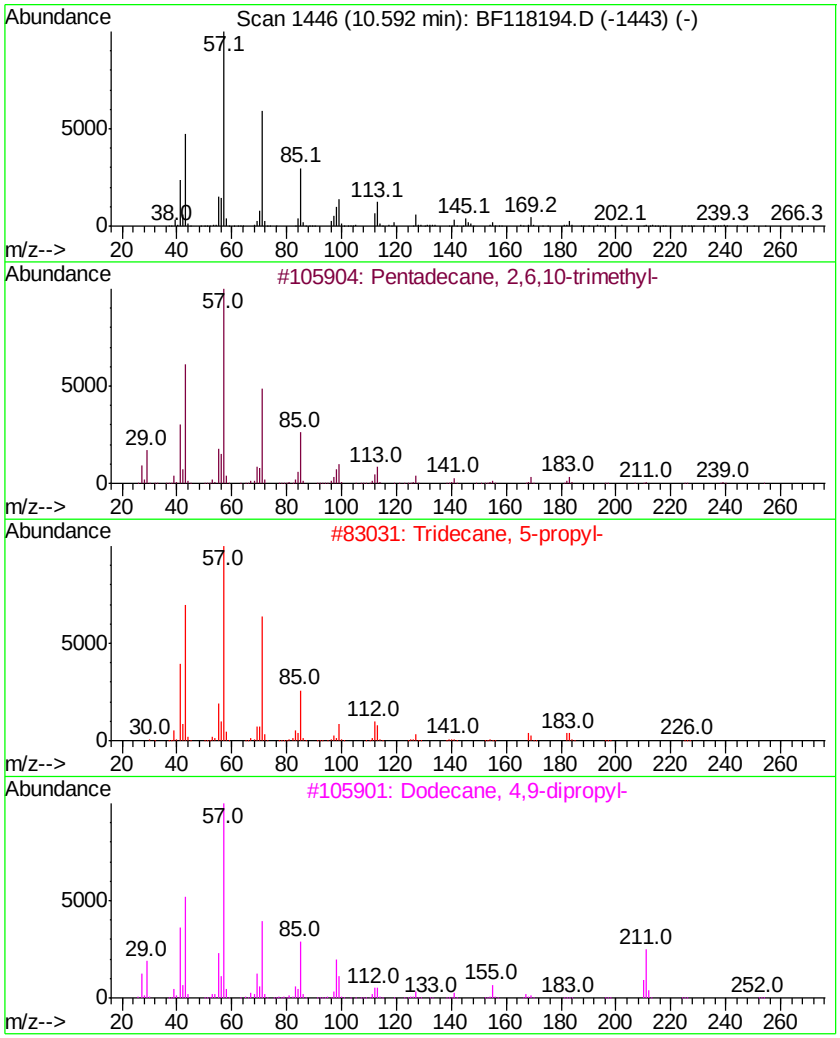
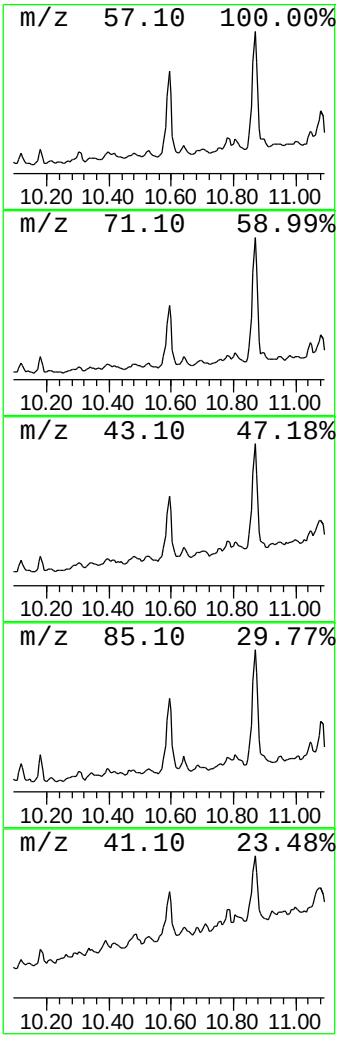
Peak Number 12 Pentadecane, 2,6,10-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	45.35 ng	3147470	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	95
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	87
3	Dodecane, 4,9-dipropyl-	254	C18H38	003054-63-5	72
4	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	64
5	Hexadecane	226	C16H34	000544-76-3	64





Library Search Compound Report

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Data File : BF118194.D
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Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
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TIC Integration Parameters: LSCINT.P

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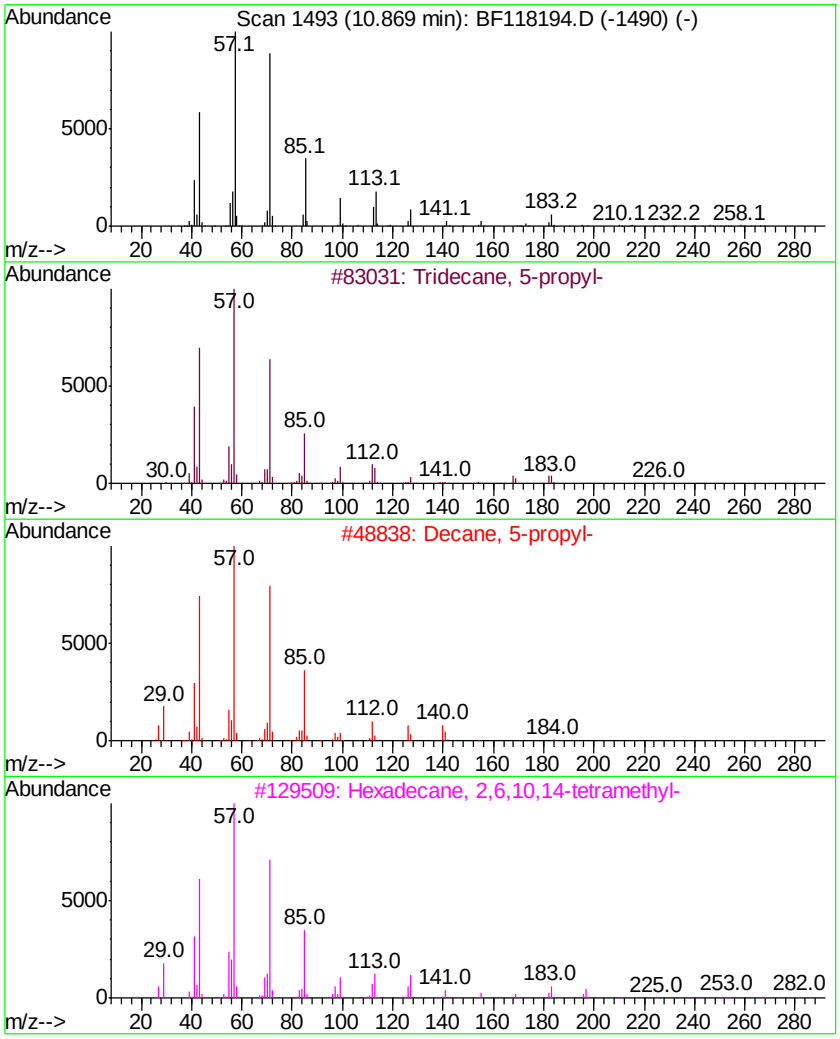
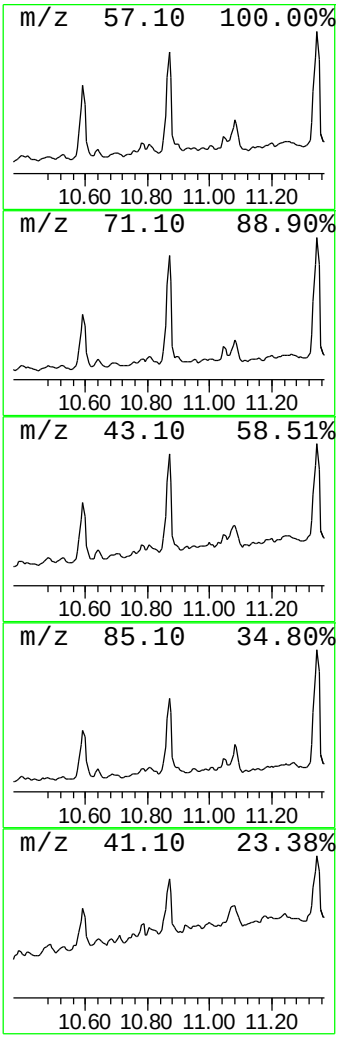
Peak Number 13 Tridecane, 5-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	20.00 ng	4995550	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 5-propyl-	226	C16H34	055045-11-9	91
2	Decane, 5-propyl-	184	C13H28	017312-62-8	80
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	59
4	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	59
5	Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	59





Library Search Compound Report

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Data File : BF118194.D
Acq On : 13 Dec 2019 18:59
Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
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TIC Library : C:\DATABASE\NIST11.L
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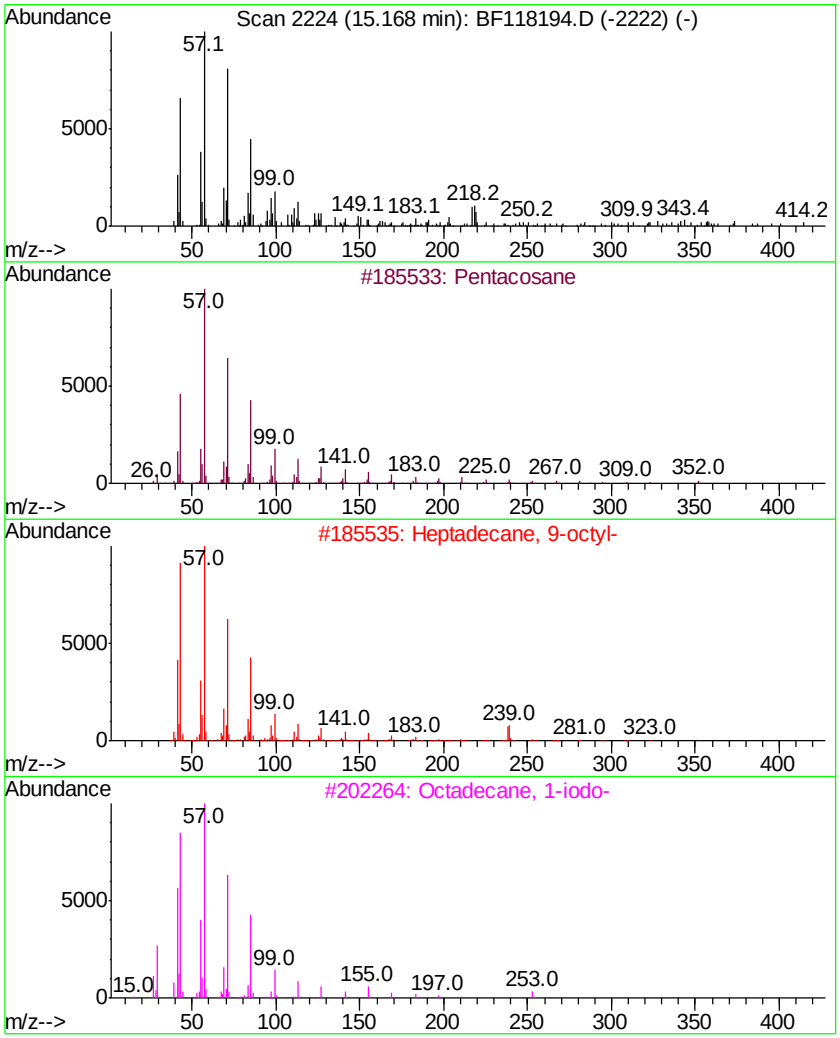
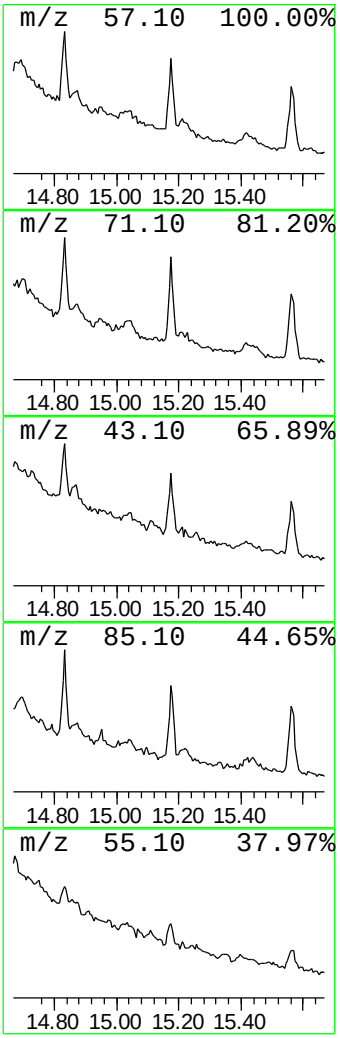
Peak Number 14 Pentacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	5.50 ng	253424	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	83





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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
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TIC Integration Parameters: LSCINT.P

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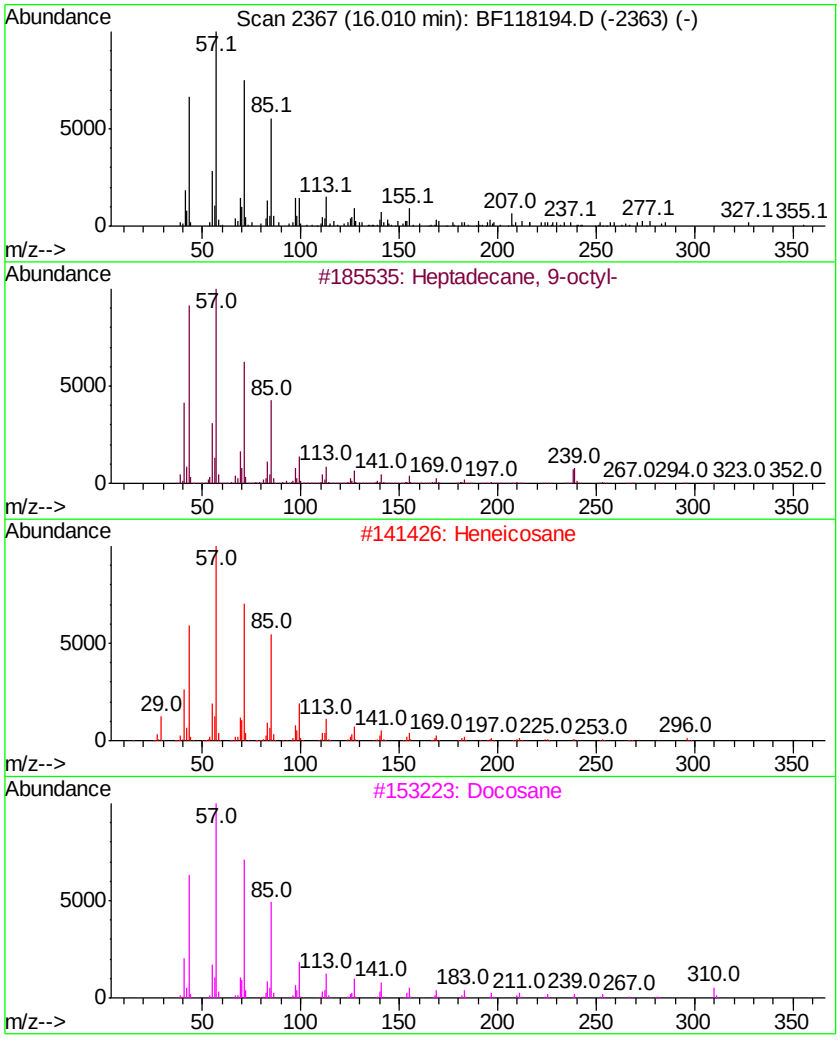
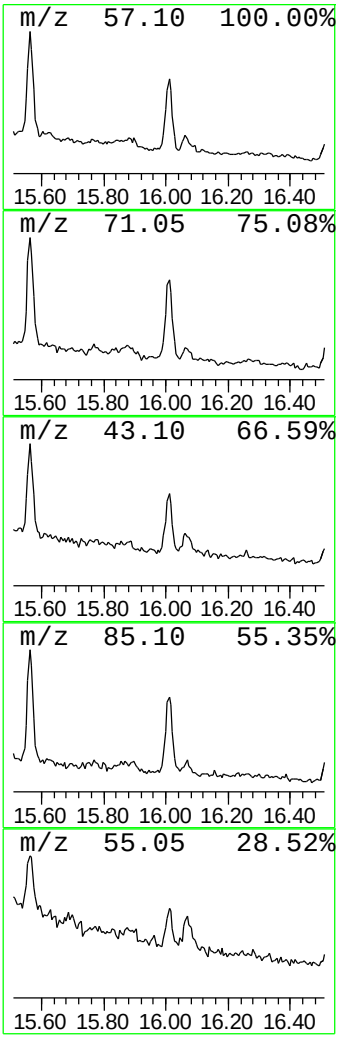
Peak Number 15 Heptadecane, 9-octyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	3.57 ng	164504	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Docosane	310	C22H46	000629-97-0	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	86





Tentatively Identified Compound (LSC) summary

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Acq On : 13 Dec 2019 18:59
Operator : JU
Sample : K6274-01
Misc :
ALS Vial : 18 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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.12	10.4	ng	333788	1	6.87	641475	20.0
2-Pentanone, 4-hy...	5.07	12.8	ng	411180	1	6.87	641475	20.0
unknown6.64	6.64	71.7	ng	2298920	1	6.87	641475	20.0
1-Dodecanol, 2-oc...	9.32	3.4	ng	238865	3	9.92	1388120	20.0
Benzene, 1-cycloh...	9.55	5.2	ng	360127	3	9.92	1388120	20.0
Cetene	9.79	9.6	ng	666626	3	9.92	1388120	20.0
unknown9.82	9.82	11.6	ng	802228	3	9.92	1388120	20.0
unknown9.86	9.86	8.2	ng	569634	3	9.92	1388120	20.0
Dodecane, 2,6,11-...	10.18	18.9	ng	1310110	3	9.92	1388120	20.0
Aromadendrene, de...	10.24	8.5	ng	588341	3	9.92	1388120	20.0
Pentadecane, 2,6,...	10.59	45.4	ng	3147470	3	9.92	1388120	20.0
Tridecane, 5-propyl-	10.87	20.0	ng	4995550	4	11.44	4995550	20.0
Pentacosane	15.17	5.5	ng	253424	6	15.56	921638	20.0
Heptadecane, 9-oc...	16.01	3.6	ng	164504	6	15.56	921638	20.0