LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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	5.357	550	556	559	rBV	3396222	3634488	85.30%	9.328%
2	6.375	724	729	734	rBV2	3801430	4100414	96.24%	10.524%
3	6.510	747	752	756	rBV	3978656	3890544	91.31%	9.985%
4	6.740	788	791	795	rBV	1243075	1123395	26.37%	2.883%
5	6.898	814	818	822	rBV	3406647	3002510	70.47%	7.706%
6	7.298	881	886	889	rBV	2445269	2463814	57.82%	6.323%
7	8.022	1005	1009	1013	rBV	1639281	1410214	33.10%	3.619%
8	8.451	1078	1082	1091	rBV	132277	145590	3.42%	0.374%
9	9.098	1188	1192	1195	rBV	4930771	4260823	100.00%	10.936%
10	9.228	1211	1214	1224	rVB2	47852	64676	1.52%	0.166%
11	9.486	1255	1258	1264	rBV	325376	294931	6.92%	0.757%
12	9.663	1285	1288	1296	rVB5	26175	48362	1.14%	0.124%
13	9.769	1303	1306	1315	rVB	1629637	1587099	37.25%	4.073%
14	10.557	1435	1440	1443	rBV	2633498	2579162	60.53%	6.619%
15	11.251	1554	1558	1561	rBV	1634121	1533960	36.00%	3.937%
16	11.463	1589	1594	1597	rBV	45310	46947	1.10%	0.120%
17	11.786	1645	1649	1653	rBV	449421	415606	9.75%	1.067%
18	12.298	1733	1736	1740	rBV	50990	48166	1.13%	0.124%
19	12.569	1778	1782	1791	rBV	131446	161931	3.80%	0.416%
20	12.710	1802	1806	1810	rBV	221007	245352	5.76%	0.630%
21	12.833	1822	1827	1830	rBV	3843947	3574554	83.89%	9.174%
22	13.416	1924	1926	1933	rVB	52813	51321	1.20%	0.132%
23	13.733	1976	1980	1986	rBV2	342079	418732	9.83%	1.075%
24	13.874	2000	2004	2007	rBV	1274657	1163895	27.32%	2.987%
25	14.063	2032	2036	2041	rBV	136886	135690	3.18%	0.348%
26	14.363	2084	2087	2092	rBV	219546	206066	4.84%	0.529%
27	14.663	2134	2138	2142	rVB	233175	241797	5.67%	0.621%
28	14.980	2188	2192	2200	rBV	257049	271708	6.38%	0.697%
29	15.280	2238	2243	2248	rVB	1025539	1198466	28.13%	3.076%
30	15.339	2249	2253	2257	rVB	207911	254319	5.97%	0.653%
31	15.745	2318	2322	2326	rBV	161037	219261	5.15%	0.563%
32	16.215	2398	2402	2410	rVB2	100686	169326	3.97%	0.435%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

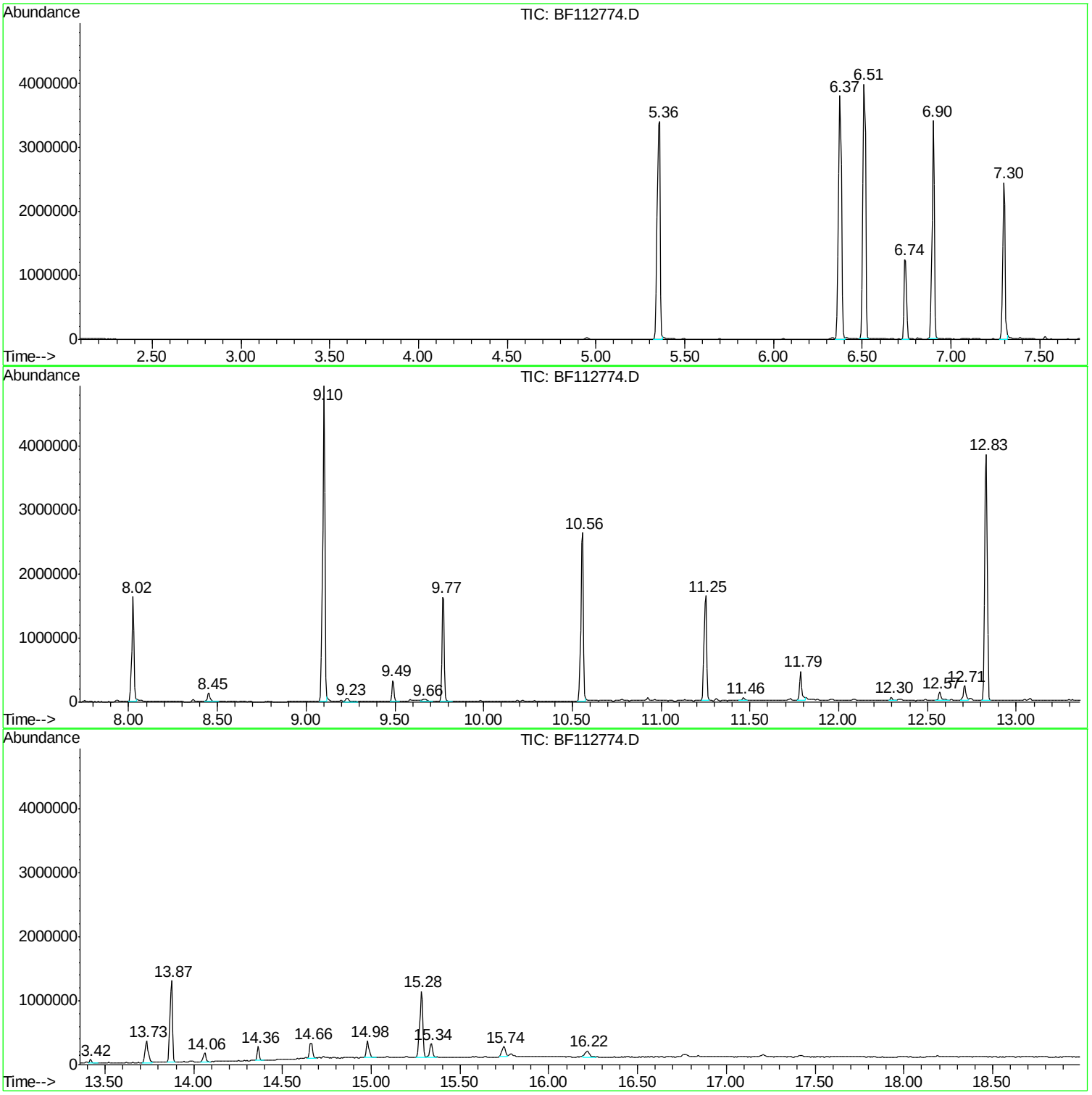
Sum of corrected areas: 38963119

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

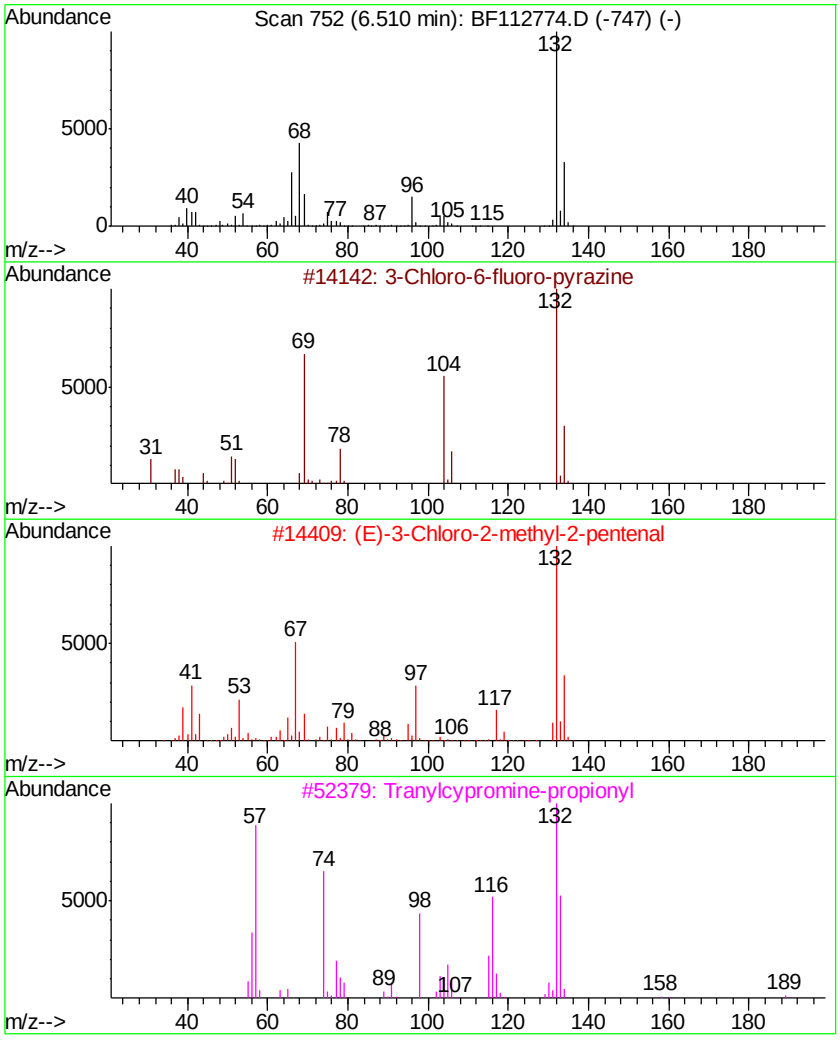
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

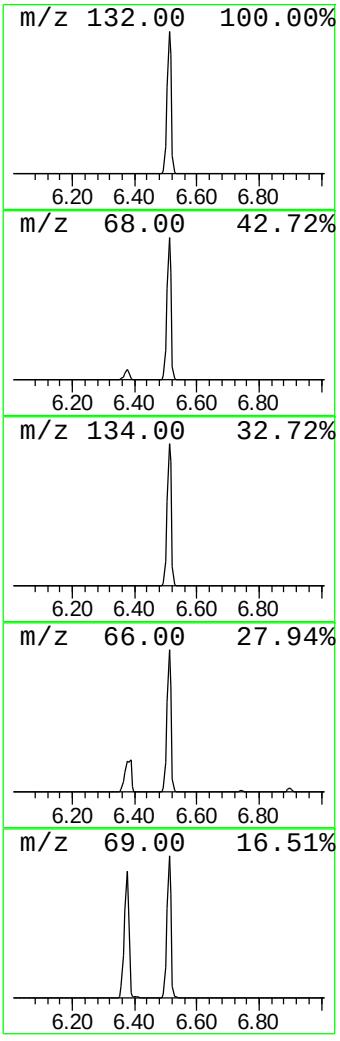
****

Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	69.26 ng	3890540	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

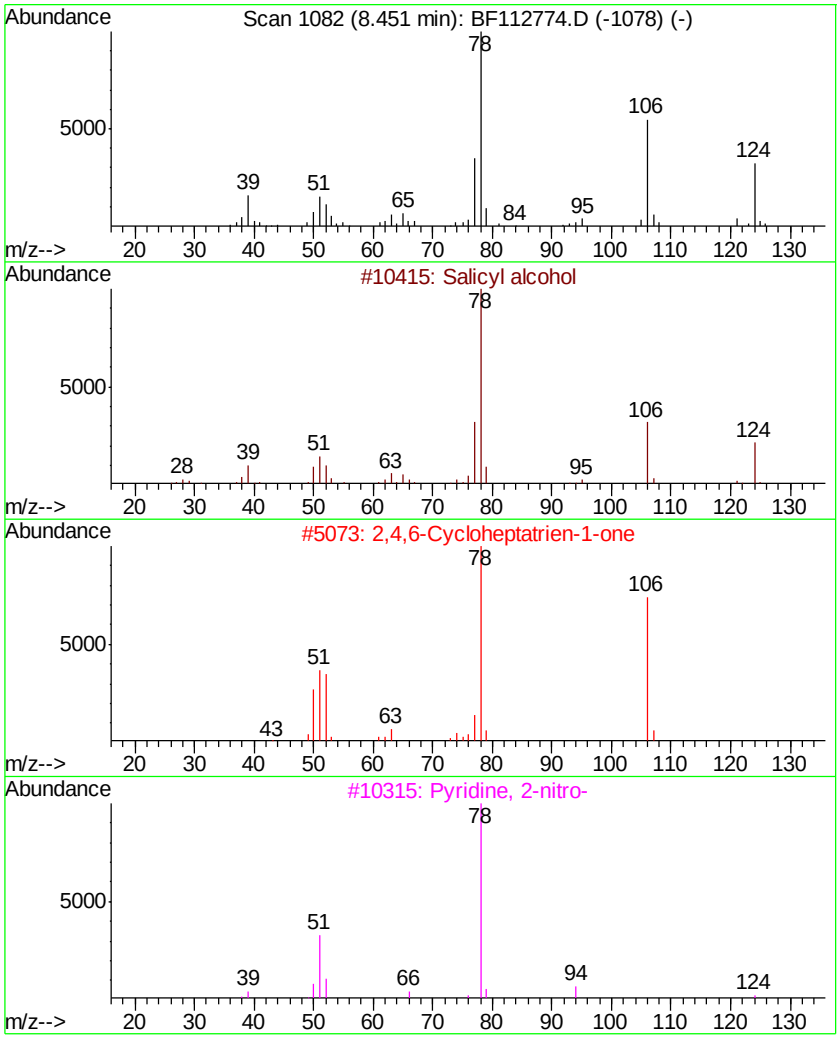
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

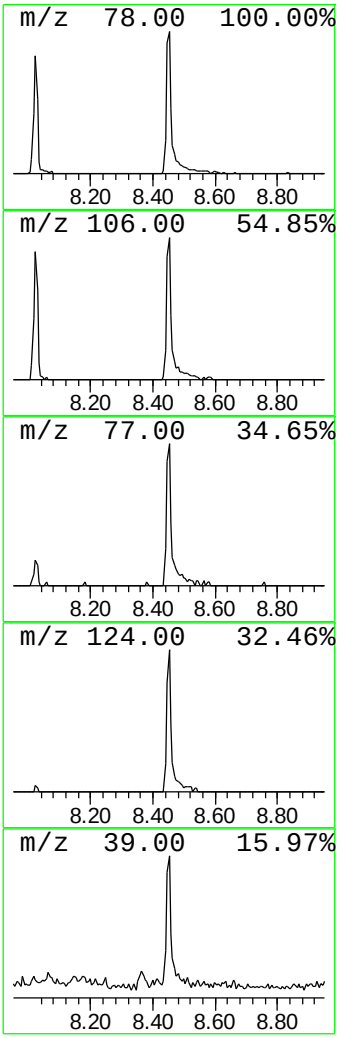
****

Peak Number 3 Salicyl alcohol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	2.06 ng	145590	Naphthalene-d8	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Salicyl alcohol	124	C7H8O2	000090-01-7	94
2	2,4,6-Cycloheptatrien-1-one	106	C7H6O	000539-80-0	90
3	Pyridine, 2-nitro-	124	C5H4N2O2	015009-91-3	64
4	2,4-Hexadiyne	78	C6H6	002809-69-0	64
5	Benzene	78	C6H6	000071-43-2	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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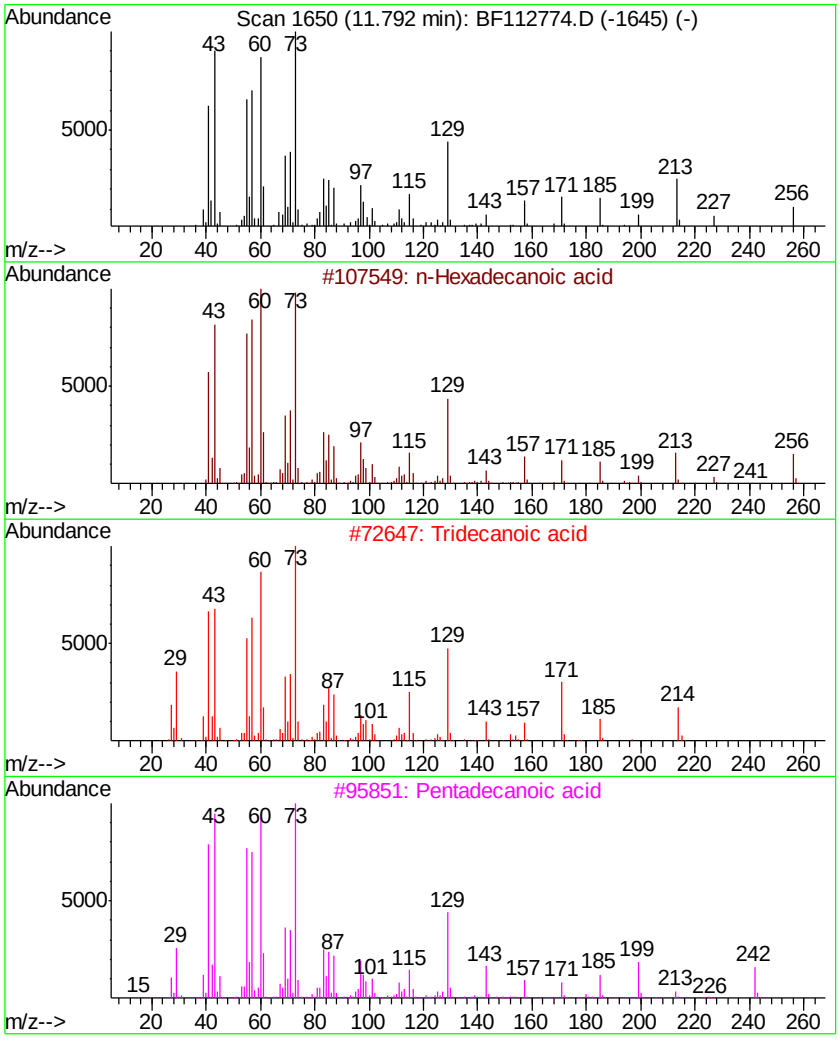
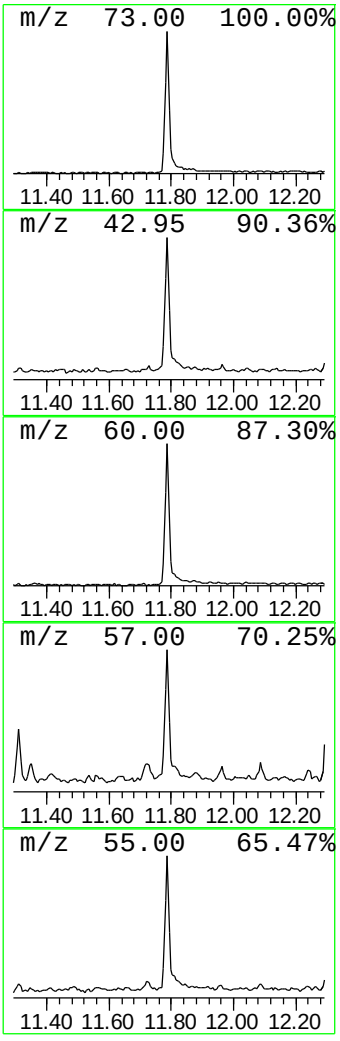
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	5.42 ng	415606	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

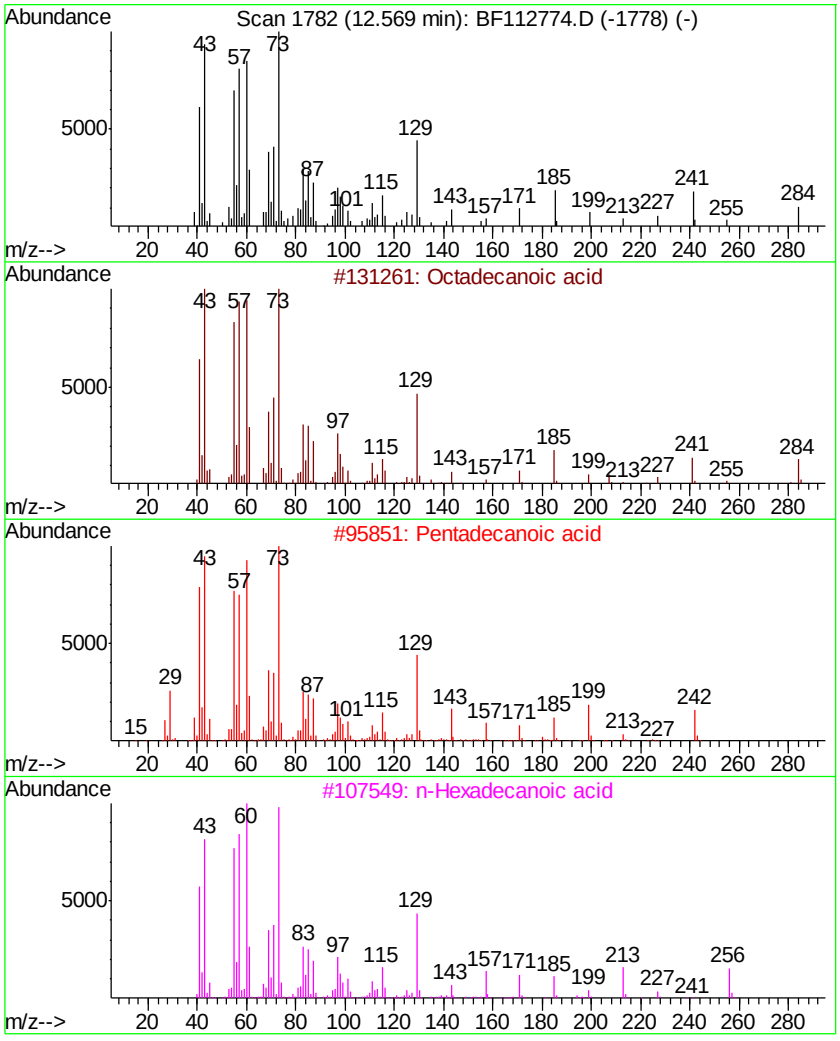
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

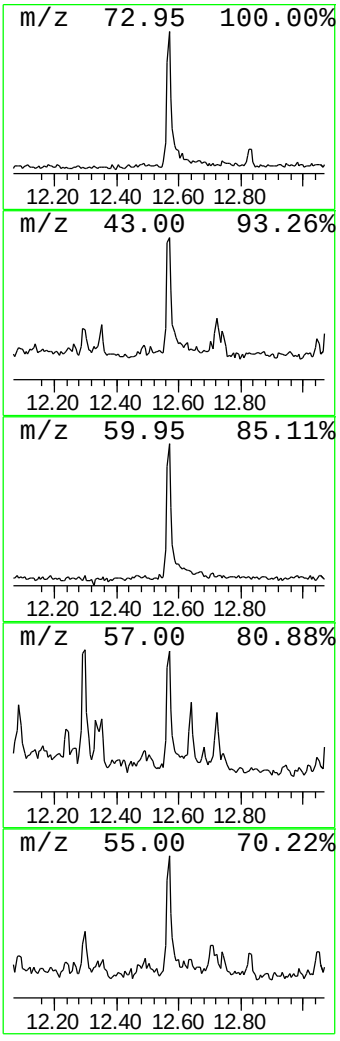
****

Peak Number 5 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	2.78 ng	161931	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

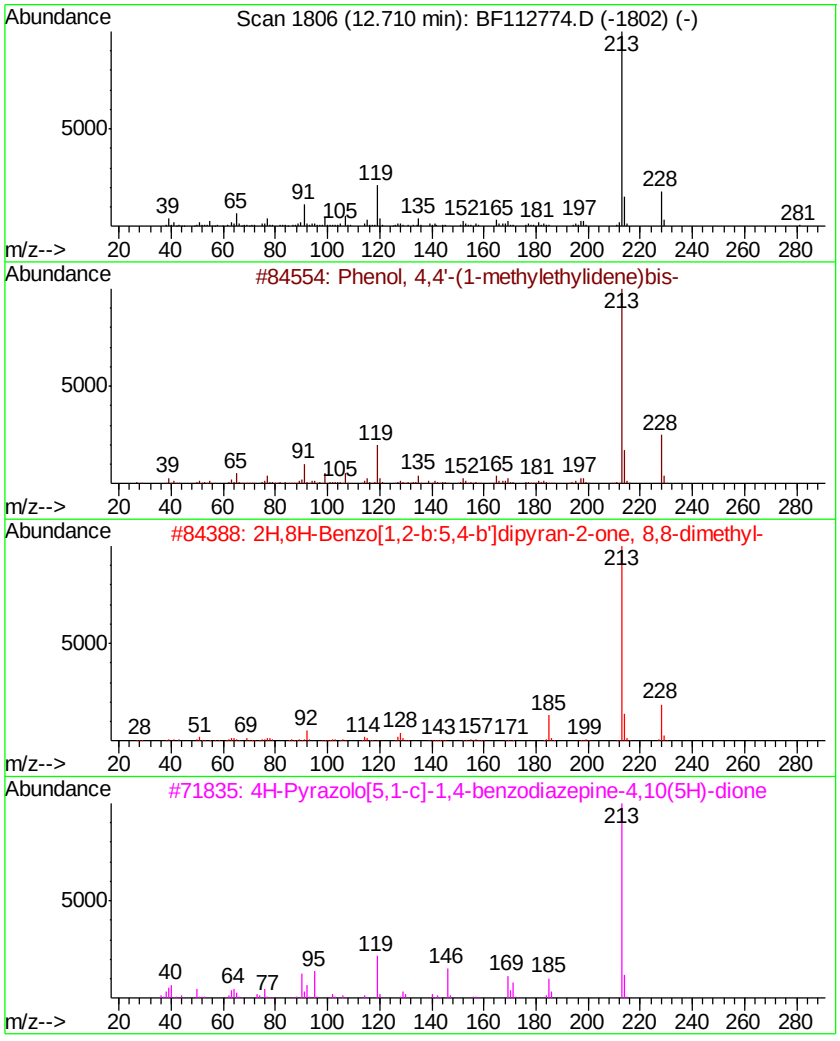
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

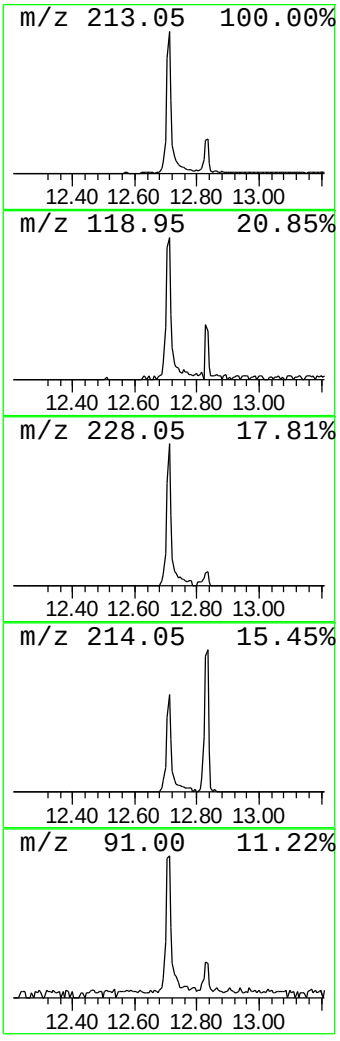
****

Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	4.22 ng	245352	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	64
3	4H-Pyrazolo[5,1-c]-1,4-benzodiaz...	213	C11H7N3O2	1000277-20-1	64
4	2,2-Bis-(4-hyxroxyphenyl)-butane	242	C16H18O2	000077-40-7	64
5	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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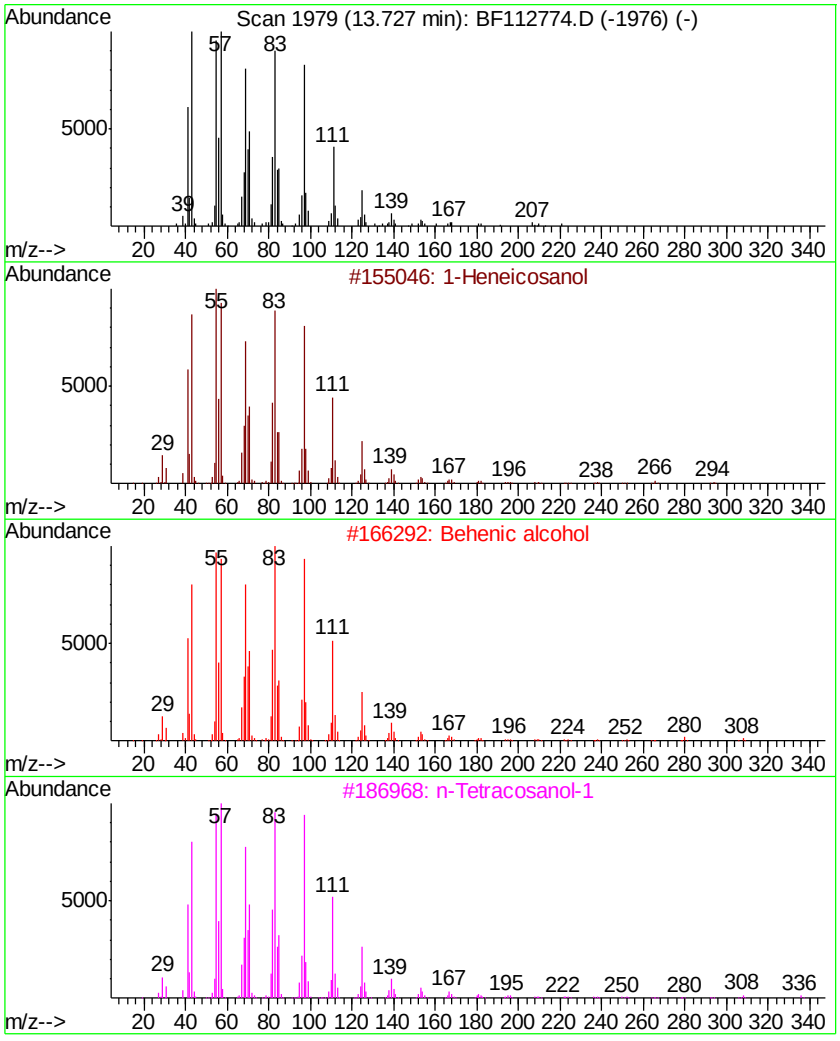
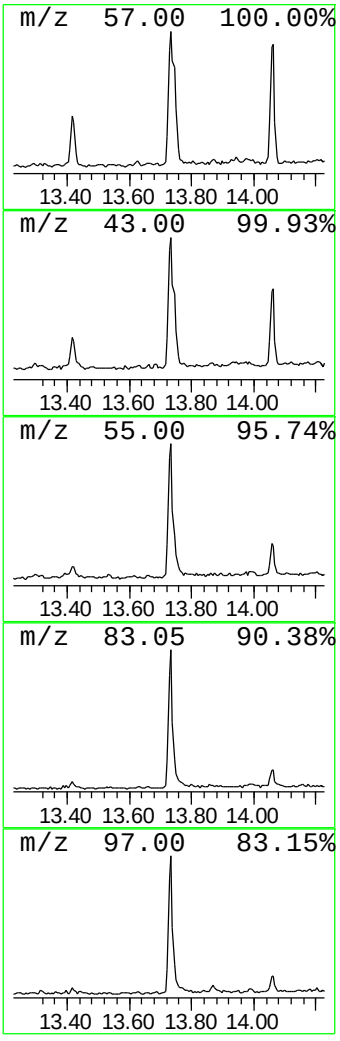
Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	7.20 ng	418732	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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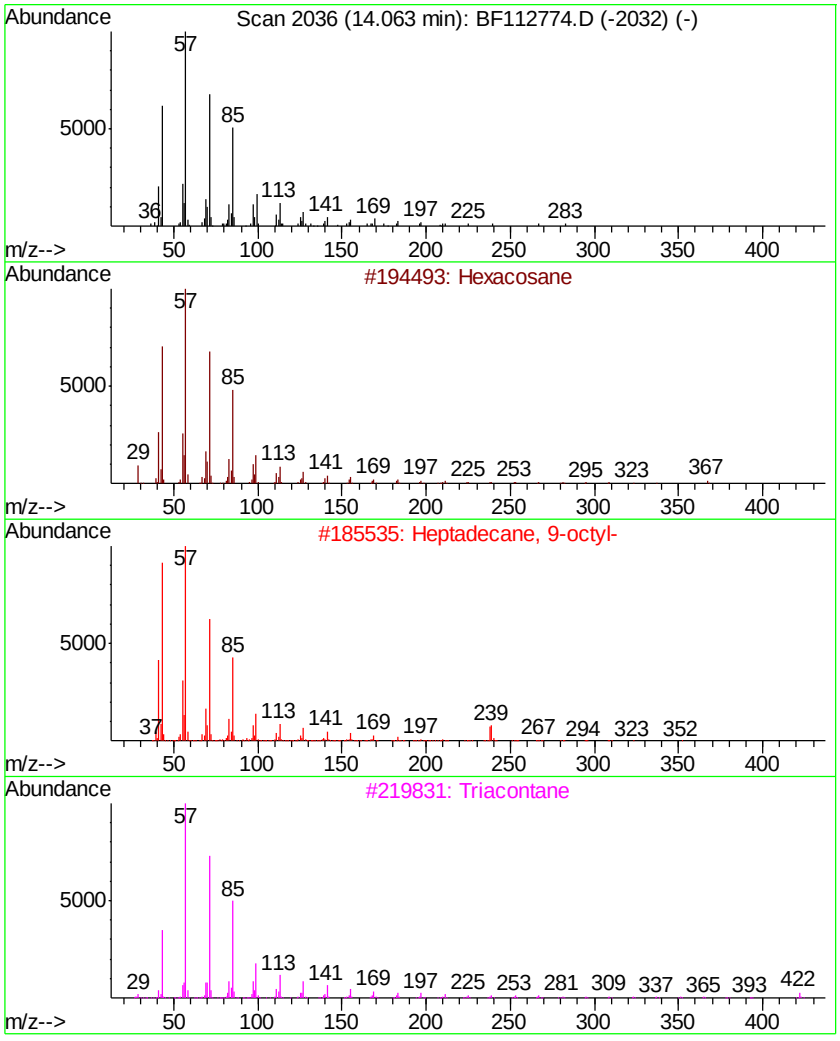
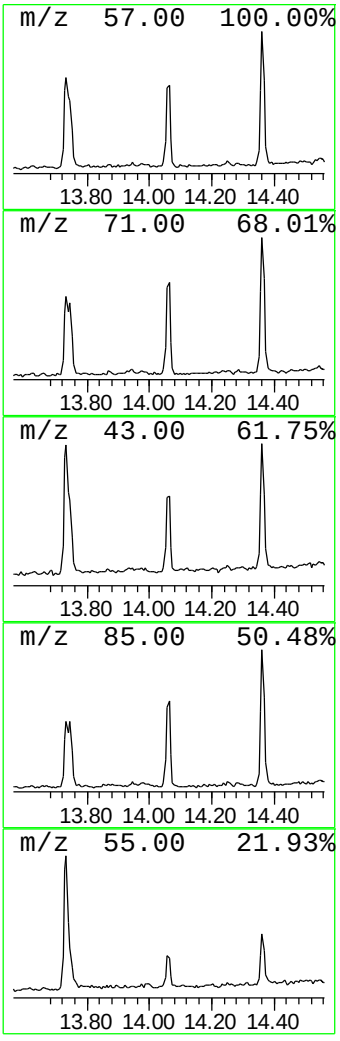
Peak Number 8 Hexacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.06	2.33 ng	135690	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
5	Tetracosane	338	C24H50	000646-31-1	90





Library Search Compound Report

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Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

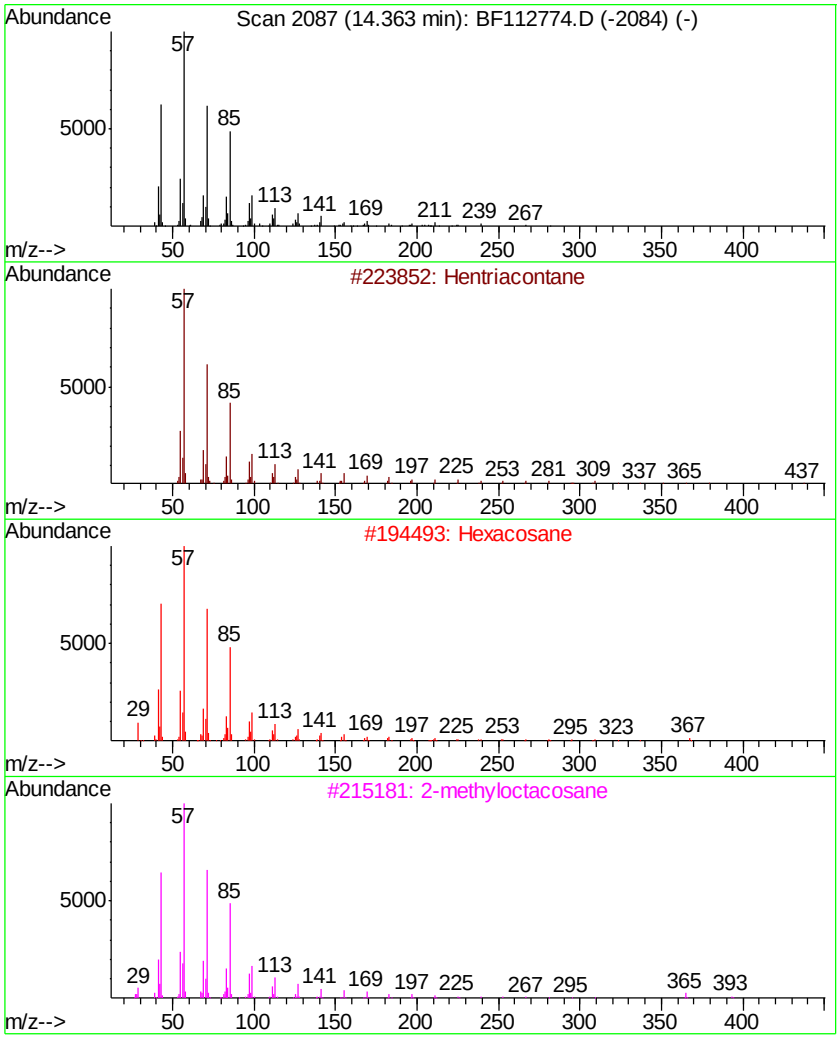
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

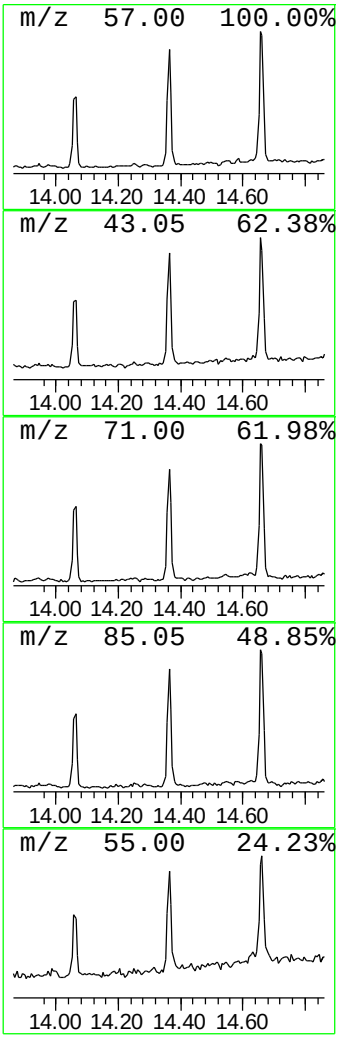
****

Peak Number 9 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	3.54 ng	206066	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Octacosane	394	C28H58	000630-02-4	90
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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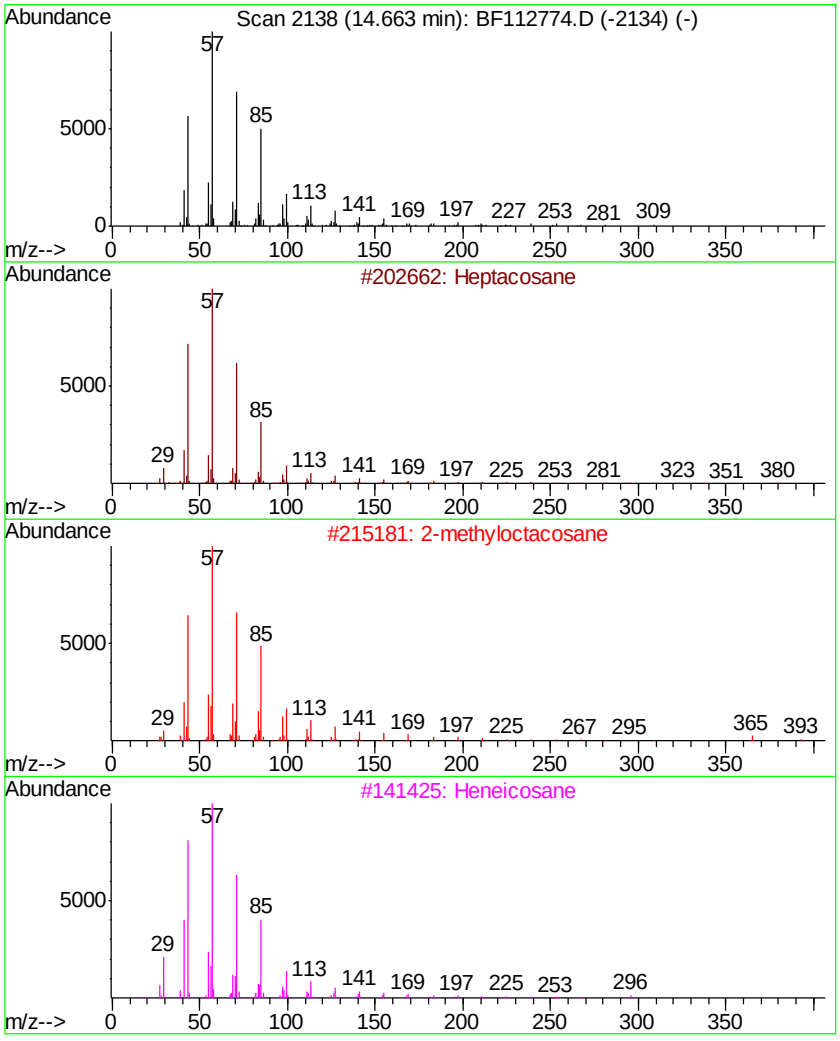
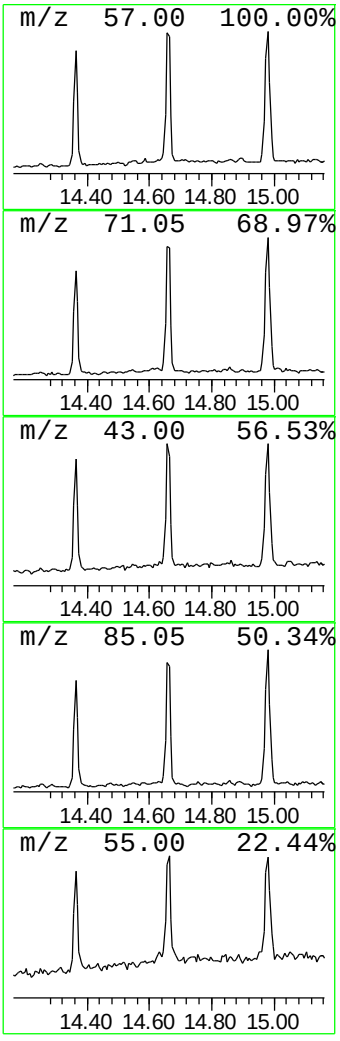
Peak Number 10 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	4.04 ng	241797	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Docosane	310	C22H46	000629-97-0	90
5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

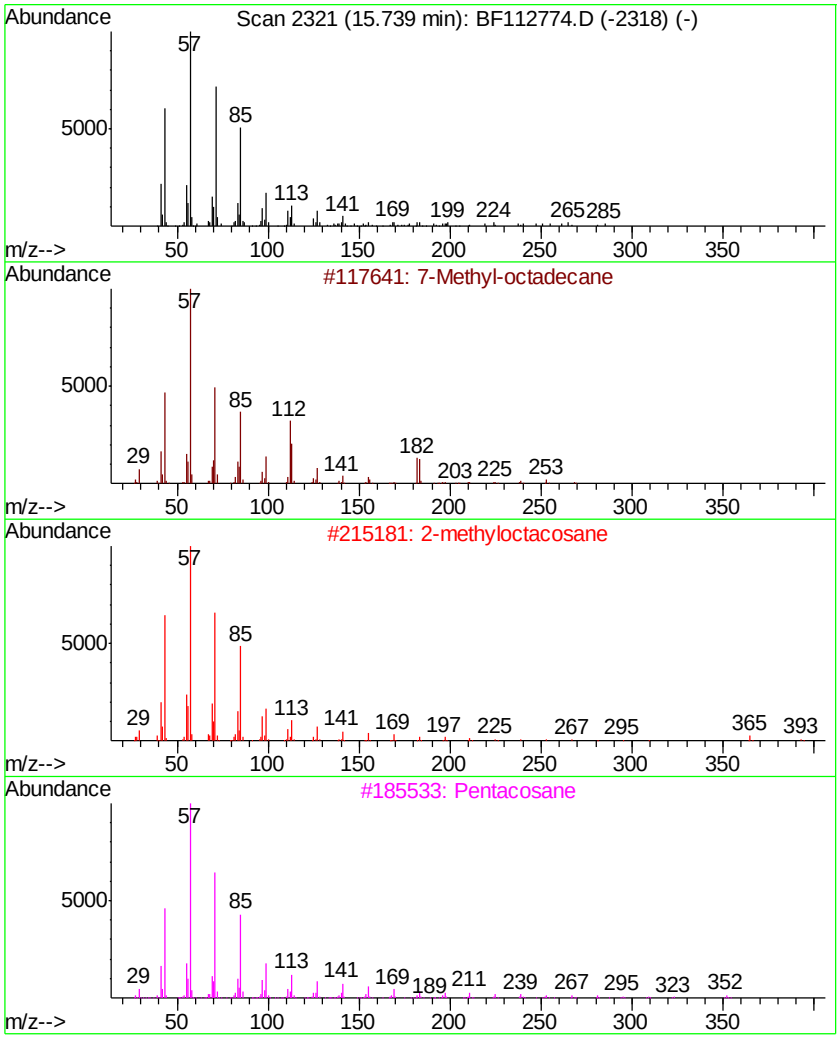
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

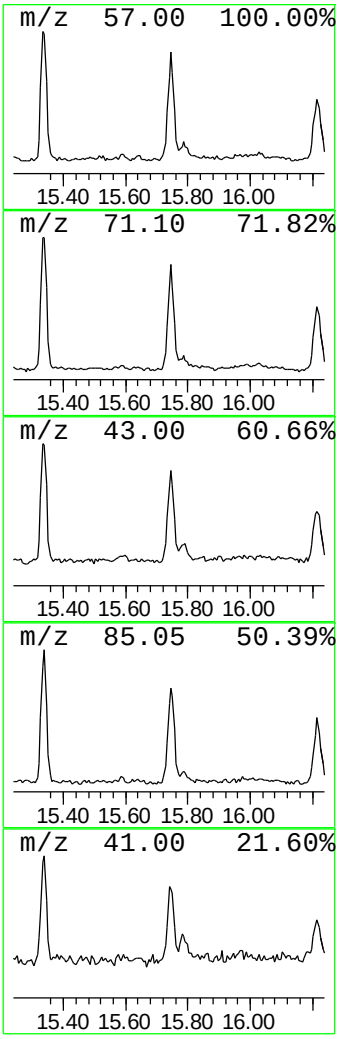
****

Peak Number 13 7-Methyl-octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	3.66 ng	219261	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methyl-octadecane	268	C19H40	1000192-63-3	87
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Pentacosane	352	C25H52	000629-99-2	86
4	Triacontane	422	C30H62	000638-68-6	86
5	Octacosane	394	C28H58	000630-02-4	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022819\
Data File : BF112774.D
Acq On : 28 Feb 2019 21:17
Operator : JU/SJ
Sample : K1650-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-7(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.51	6.51	69.3	ng	3890540	1	6.75	1123400	20.0
Salicyl alcohol	8.45	2.1	ng	145590	2	8.02	1410210	20.0
n-Hexadecanoic acid	11.79	5.4	ng	415606	4	11.25	1533960	20.0
Octadecanoic acid	12.57	2.8	ng	161931	5	13.87	1163900	20.0
Phenol, 4,4'-(1-m...	12.71	4.2	ng	245352	5	13.87	1163900	20.0
1-Heneicosanol	13.73	7.2	ng	418732	5	13.87	1163900	20.0
Hexacosane	14.06	2.3	ng	135690	5	13.87	1163900	20.0
Hentriacontane	14.36	3.5	ng	206066	5	13.87	1163900	20.0
Heptacosane	14.66	4.0	ng	241797	6	15.28	1198470	20.0
7-Methyl-octadecane	15.74	3.7	ng	219261	6	15.28	1198470	20.0