LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072418\
Data File : BF107640.D
Acq On : 25 Jul 2018 2:38
Operator : JU/SJ
Sample : J4120-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-4

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-BF072018.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	5.225	487	491	508	rBV	725759	1335293	17.56%	2.079%
2	5.613	552	557	588	rBV	5216008	7604395	100.00%	11.840%
3	6.613	721	727	745	rBV	4682210	7432050	97.73%	11.572%
4	6.748	745	750	773	rVB	5572155	7428858	97.69%	11.567%
5	6.966	784	787	809	rVB	1325457	1714767	22.55%	2.670%
6	7.125	809	814	840	rBV	5036584	5862522	77.09%	9.128%
7	7.537	878	884	908	rBV	3661125	4915019	64.63%	7.653%
8	8.248	1001	1005	1023	rBV	1855684	2056961	27.05%	3.203%
9	9.325	1182	1188	1204	rBV	6311562	7099930	93.37%	11.055%
10	9.713	1251	1254	1264	rVB	595789	528030	6.94%	0.822%
11	10.007	1300	1304	1316	rBV2	1849848	1899597	24.98%	2.958%
12	10.807	1435	1440	1452	rBV	3295541	3833695	50.41%	5.969%
13	10.895	1452	1455	1460	rVB	51579	78987	1.04%	0.123%
14	11.501	1554	1558	1567	rBV	1574880	1768045	23.25%	2.753%
15	12.007	1640	1644	1647	rBV	209195	218912	2.88%	0.341%
16	12.719	1761	1765	1770	rBV	76229	81757	1.08%	0.127%
17	12.954	1799	1805	1810	rBV3	106565	207510	2.73%	0.323%
18	13.089	1823	1828	1839	rBV	4982283	5185561	68.19%	8.074%
19	13.295	1858	1863	1867	rVB2	98493	108083	1.42%	0.168%
20	13.636	1917	1921	1924	rBV2	141544	142396	1.87%	0.222%
21	13.971	1974	1978	1990	rBV	608957	764677	10.06%	1.191%
22	14.154	2004	2009	2020	rBV	1400089	1581576	20.80%	2.463%
23	14.283	2028	2031	2034	rBV	208377	184232	2.42%	0.287%
24	14.589	2080	2083	2086	rBV	198047	191375	2.52%	0.298%
25	14.913	2133	2138	2144	rBV2	199173	239884	3.15%	0.374%
26	15.265	2195	2198	2203	rVB	164252	186030	2.45%	0.290%
27	15.313	2203	2206	2211	rBV3	61267	87303	1.15%	0.136%
28	15.689	2263	2270	2277	rBV2	777125	1282040	16.86%	1.996%
29	16.136	2341	2346	2351	rVB	132687	205891	2.71%	0.321%

Sum of corrected areas: 64225376

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072418\
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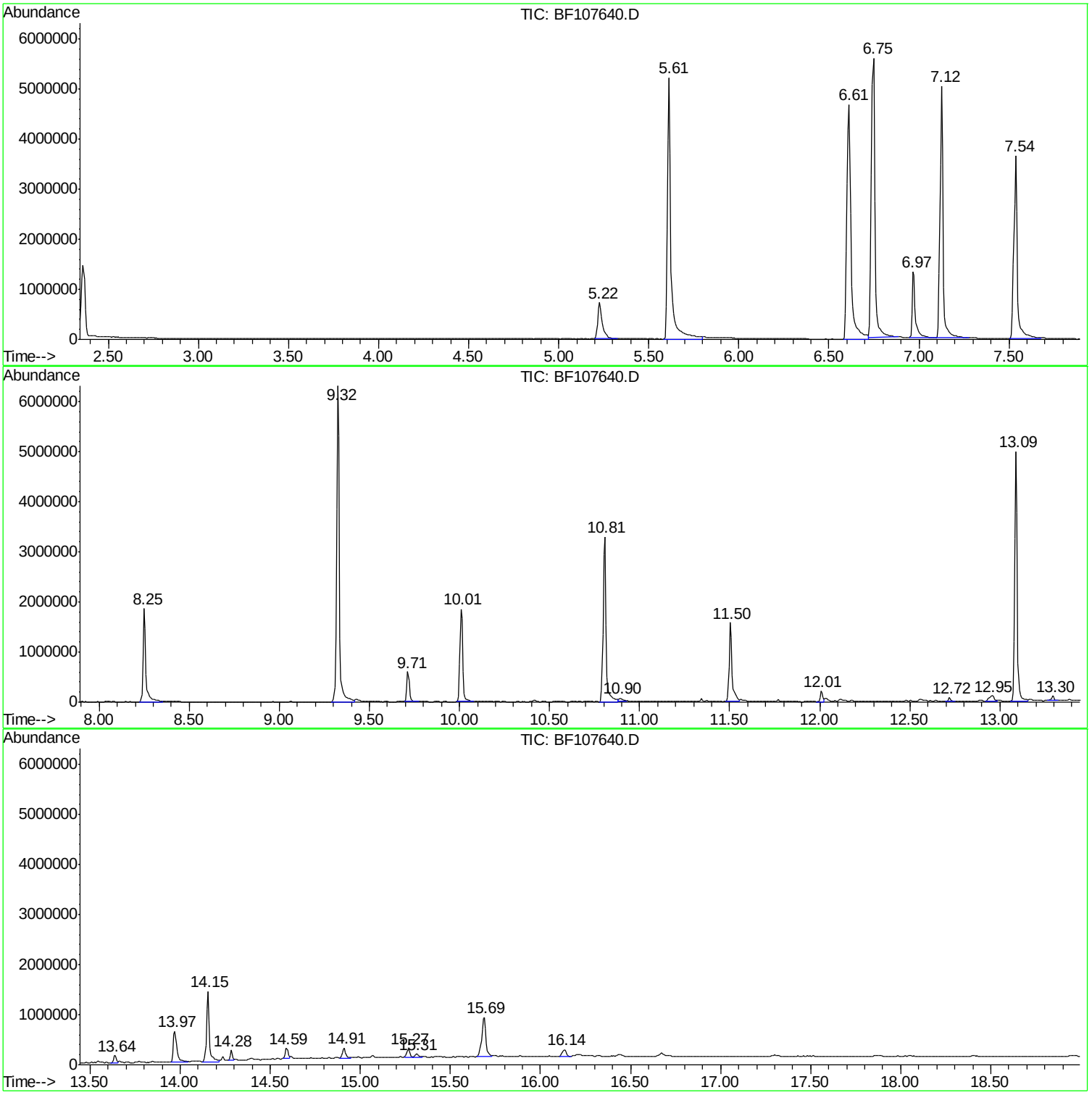
Operator : JU/SJ
Sample : J4120-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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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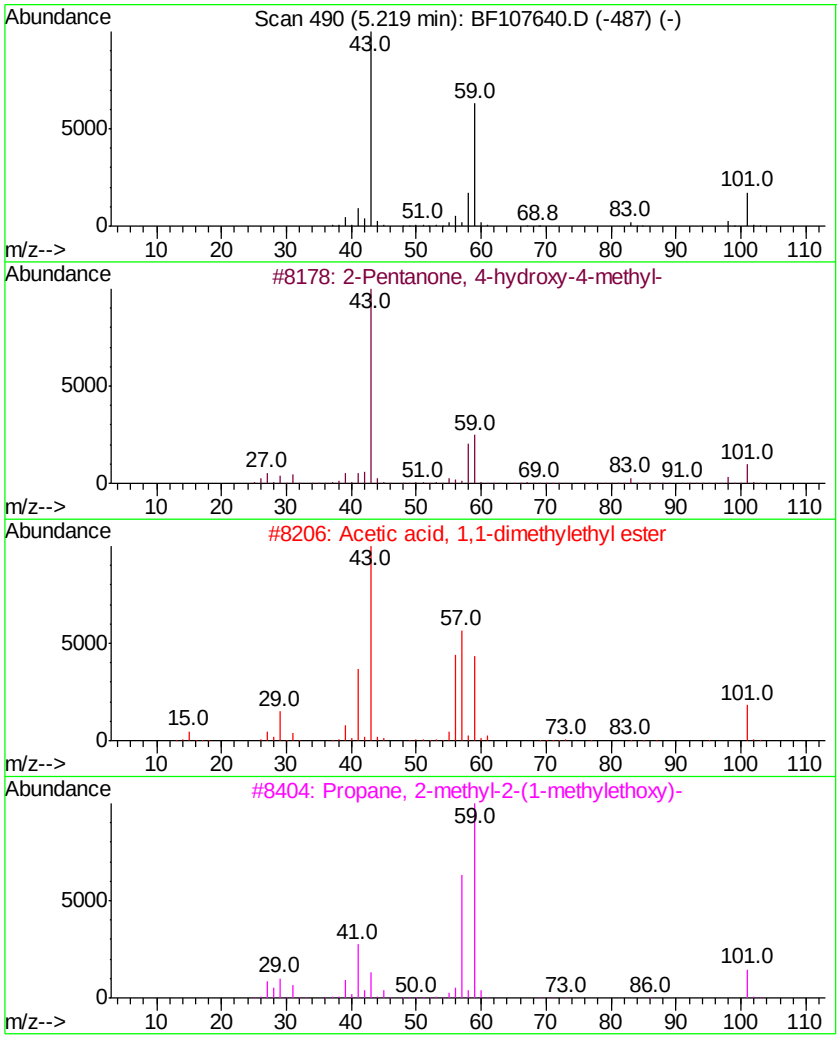
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

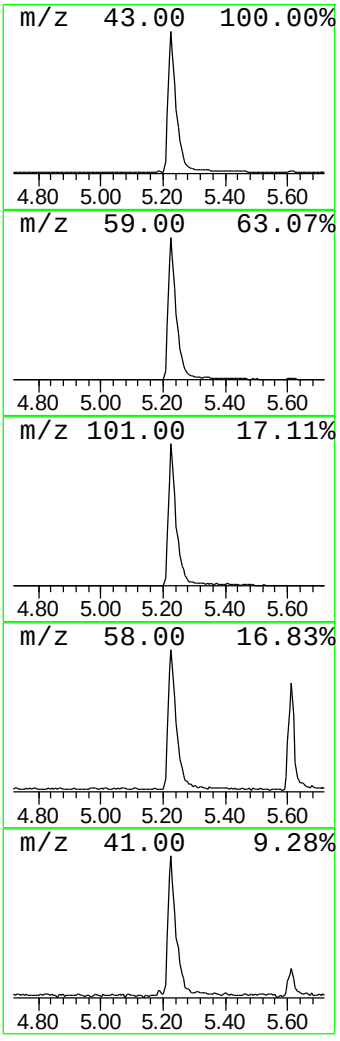
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	15.57 ng	1335290	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Library Search Compound Report

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Acq On : 25 Jul 2018 2:38
Operator : JU/SJ
Sample : J4120-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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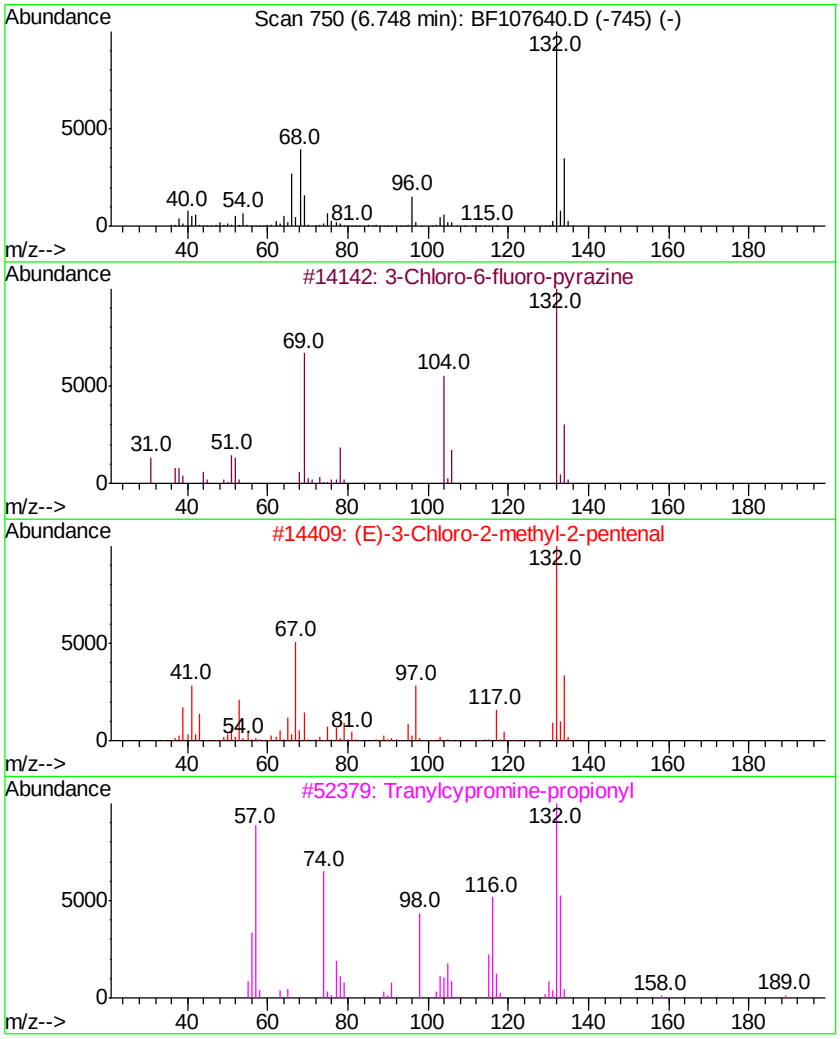
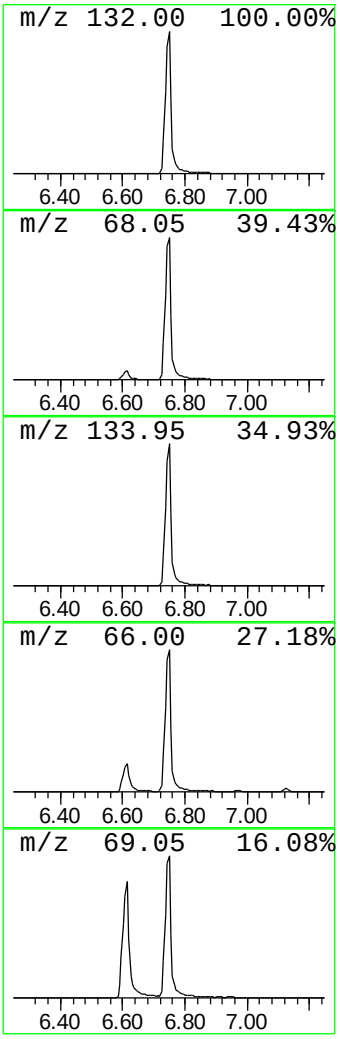
Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	86.65 ng	7428860	1,4-Dichlorobenzene-d4	6.97

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	10
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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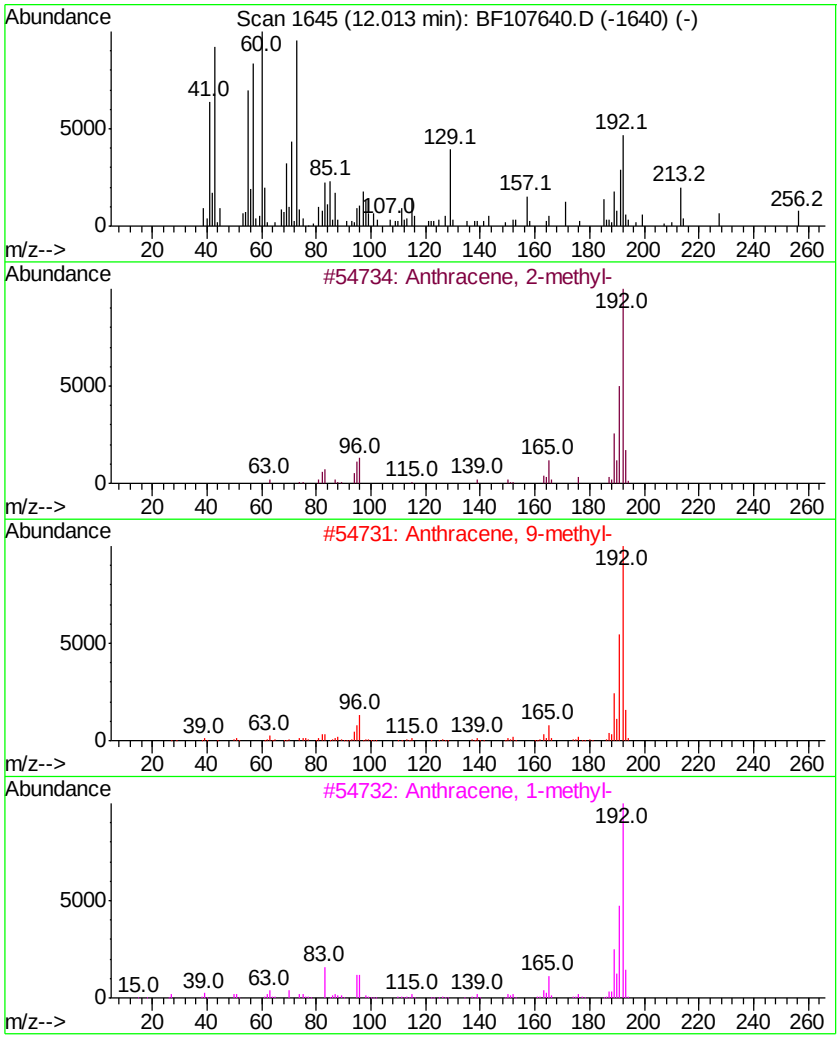
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

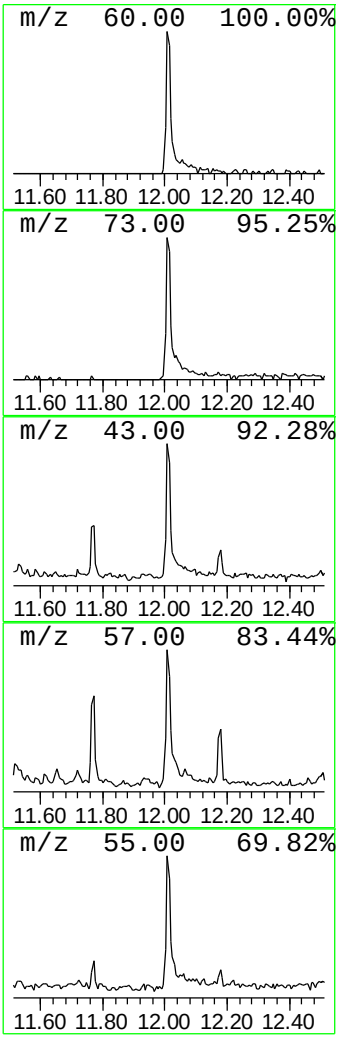
****

Peak Number 4 Anthracene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.48 ng	218912	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	84
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	64
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	60





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Sample : J4120-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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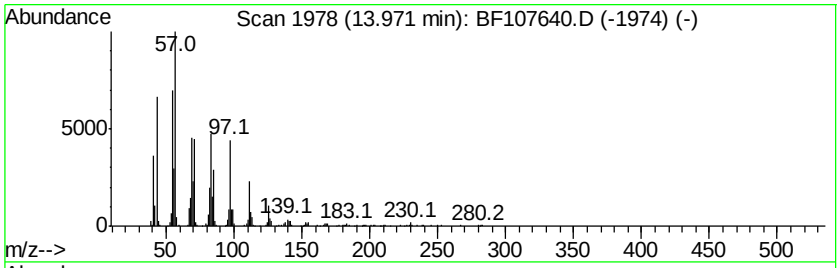
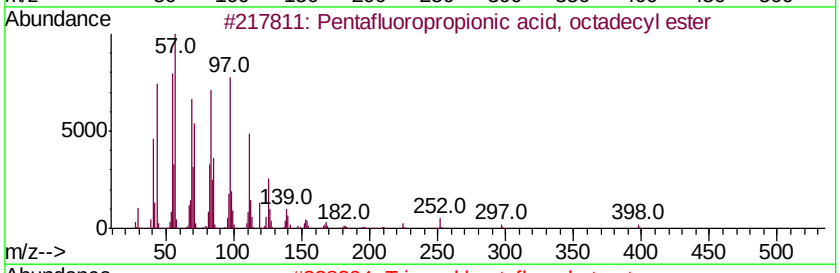
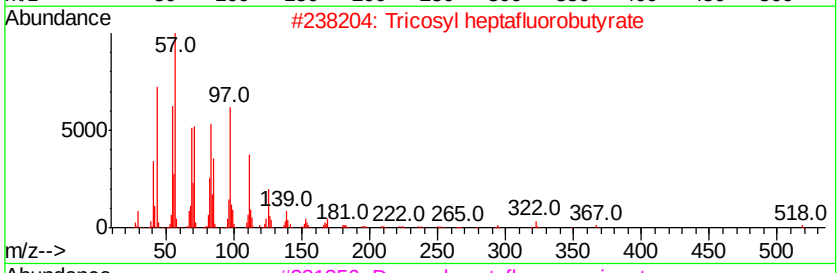
Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

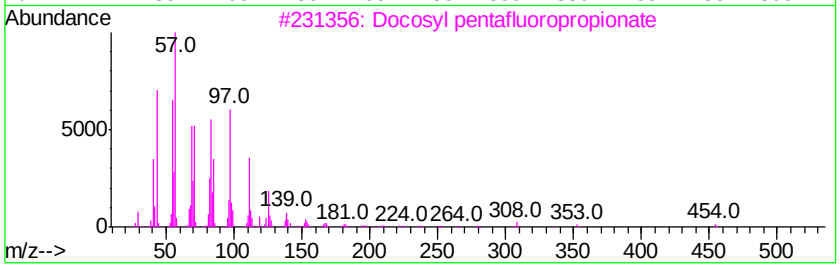
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	9.67 ng	764677	Chrysene-d12	14.15

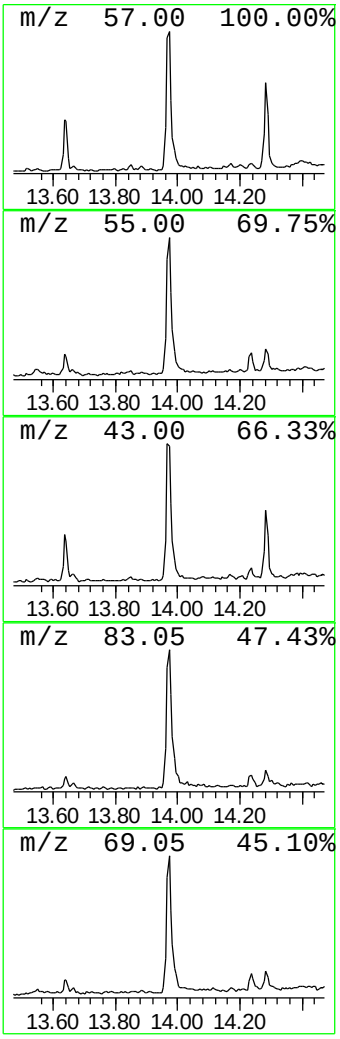
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91











Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072418\
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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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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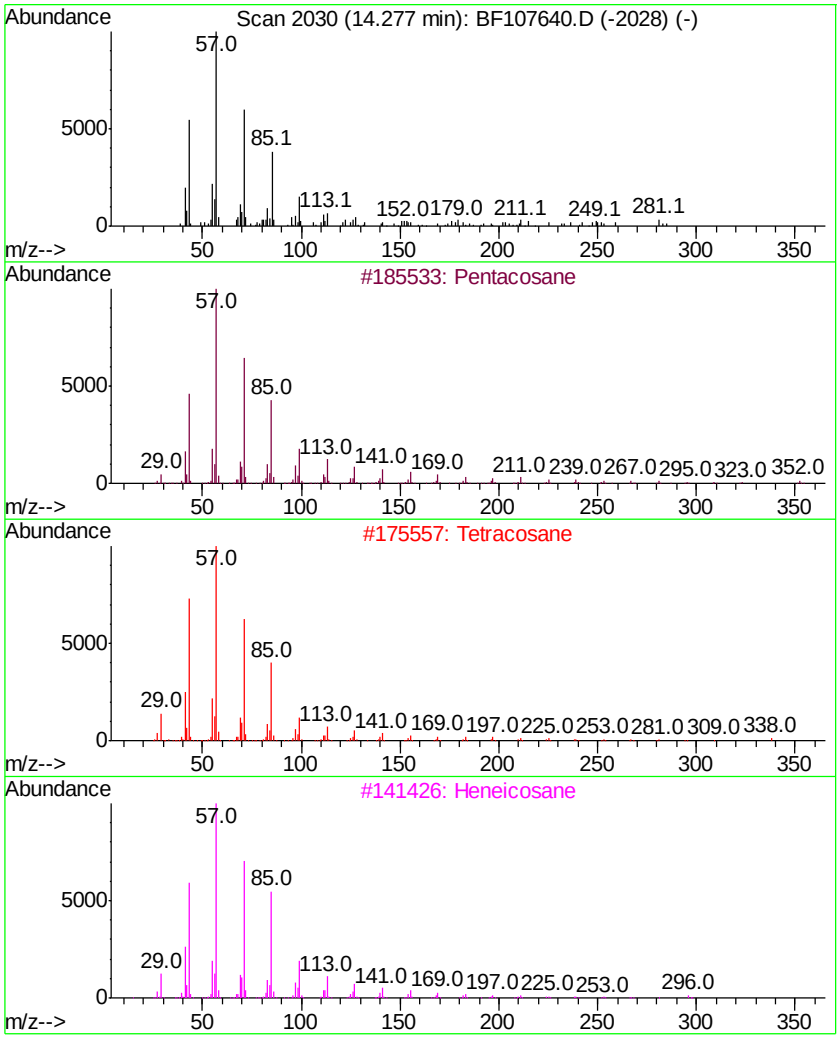
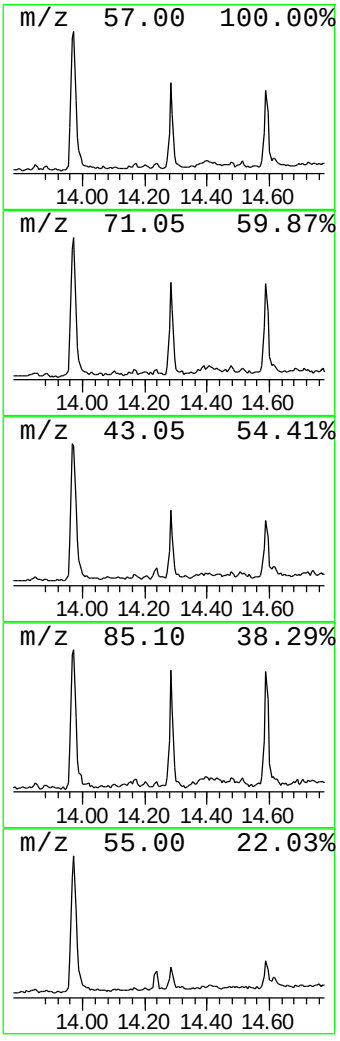
Peak Number 7 Pentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	2.33 ng	184232	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Tetracosane	338	C24H50	000646-31-1	87
3	Heneicosane	296	C21H44	000629-94-7	83
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5	Heptacosane	380	C27H56	000593-49-7	74





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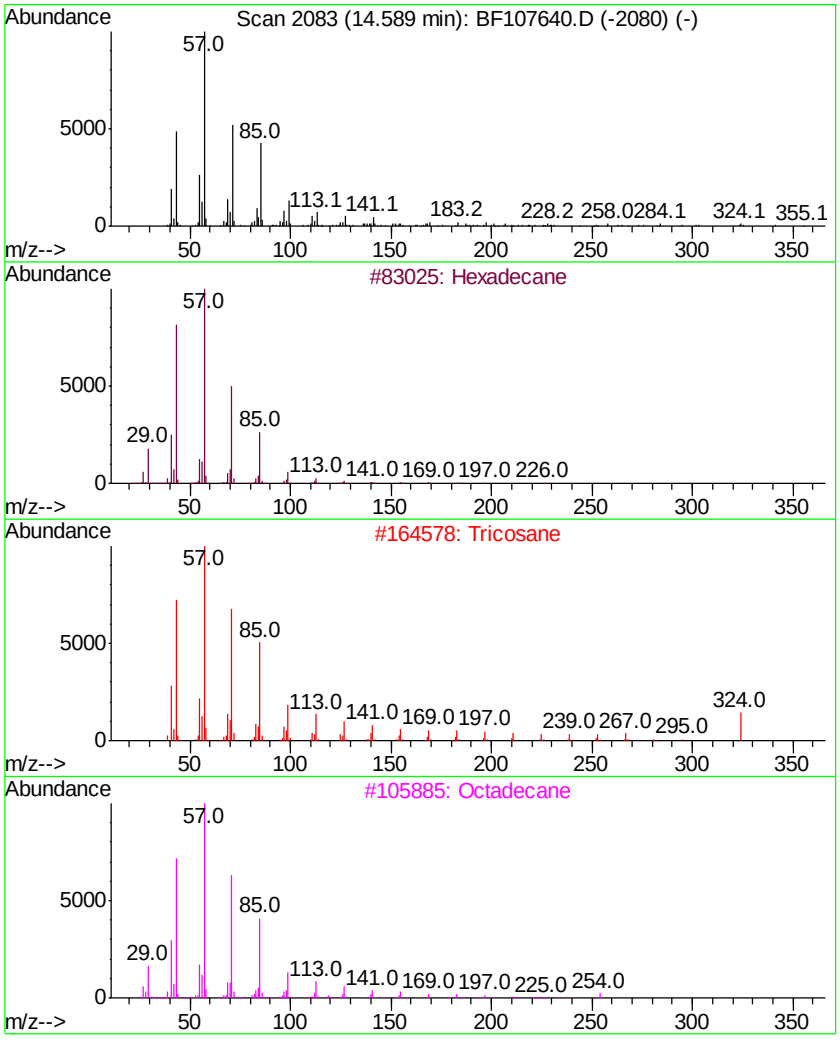
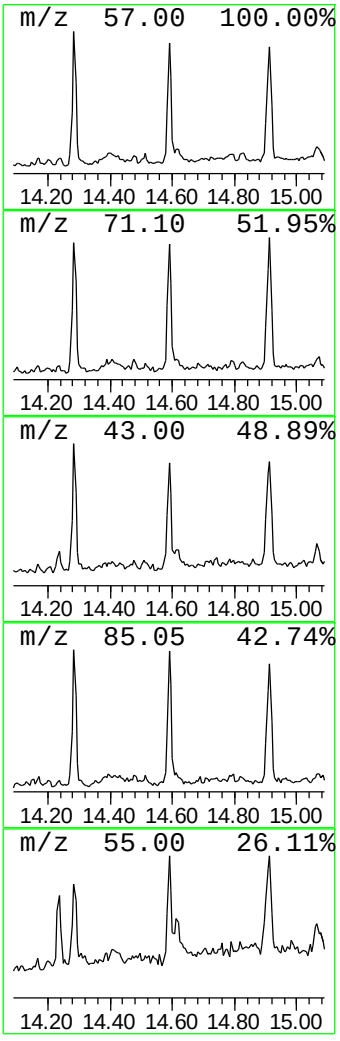
Peak Number 8 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.42 ng	191375	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Tricosane	324	C23H48	000638-67-5	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Pentacosane	352	C25H52	000629-99-2	90
5	Eicosane	282	C20H42	000112-95-8	90





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Operator : JU/SJ
Sample : J4120-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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TIC Library : C:\DATABASE\NIST11.L
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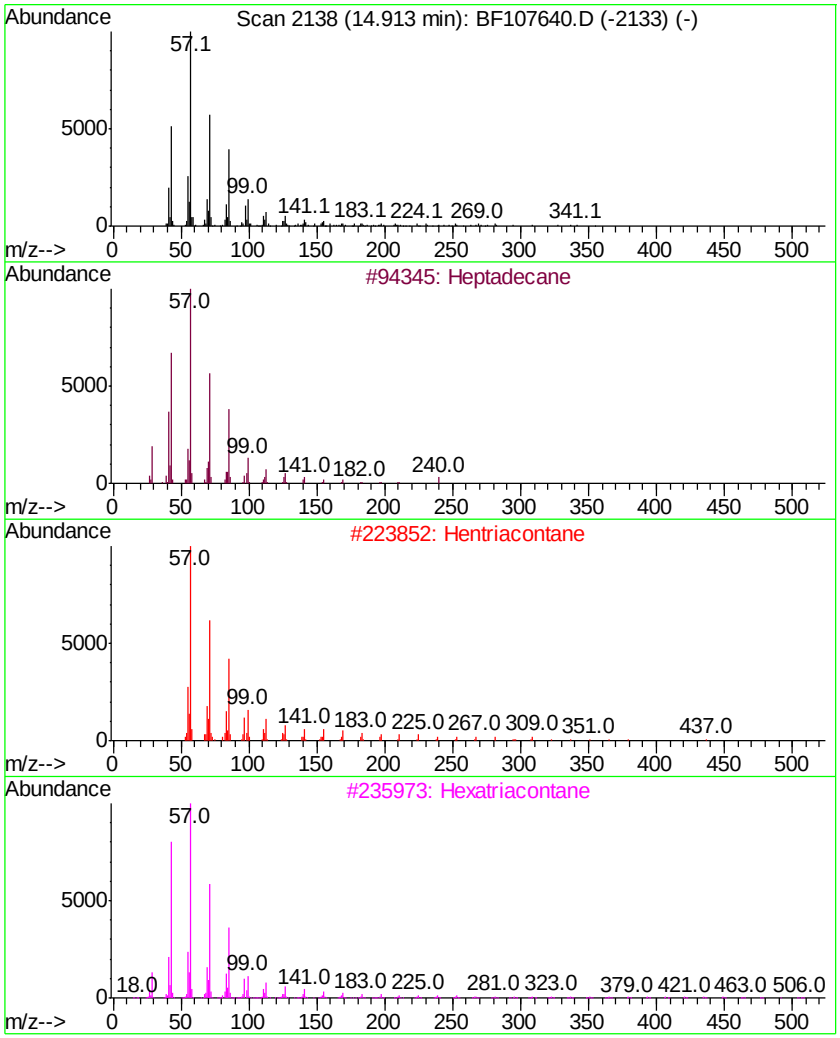
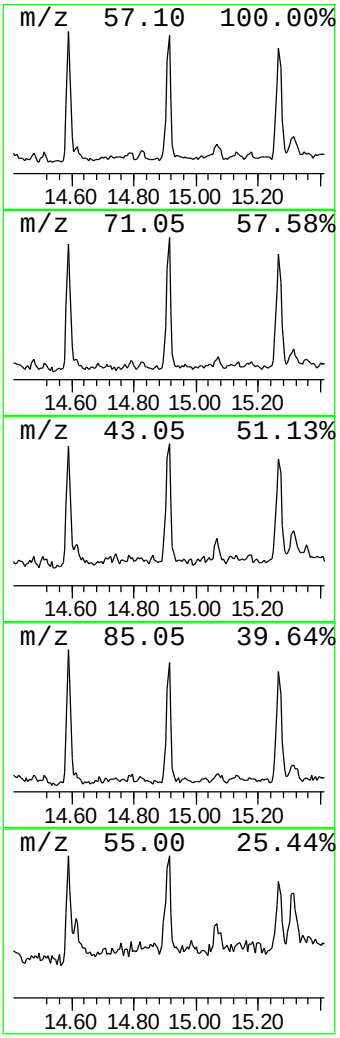
Peak Number 9 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	3.03 ng	239884	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Hexatriacontane	507	C36H74	000630-06-8	87
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
5	Tetracosane	338	C24H50	000646-31-1	86





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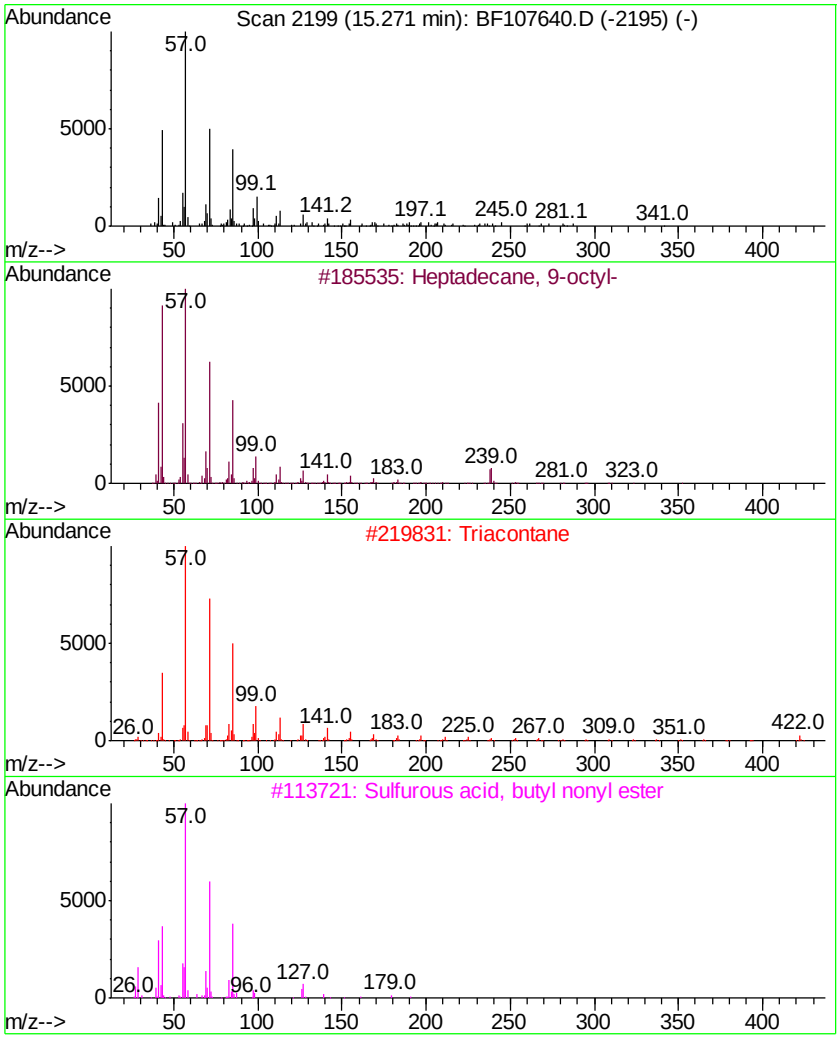
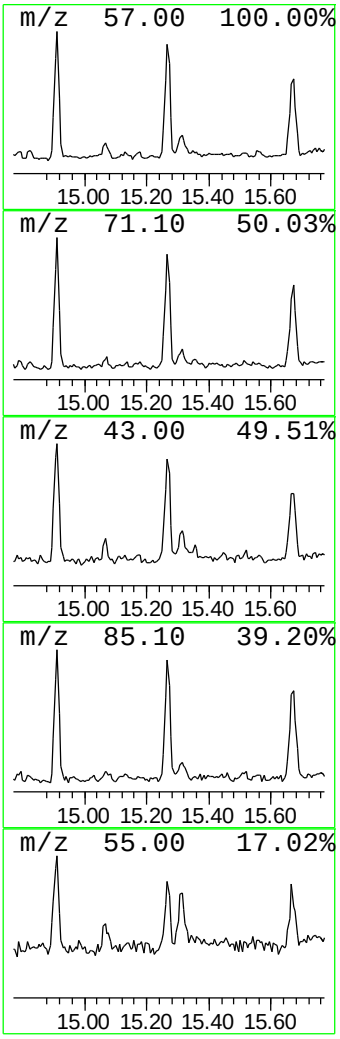
Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	2.90 ng	186030	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
2	Triacontane	422	C30H62	000638-68-6	80
3	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	72
4	Eicosane	282	C20H42	000112-95-8	72
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	72





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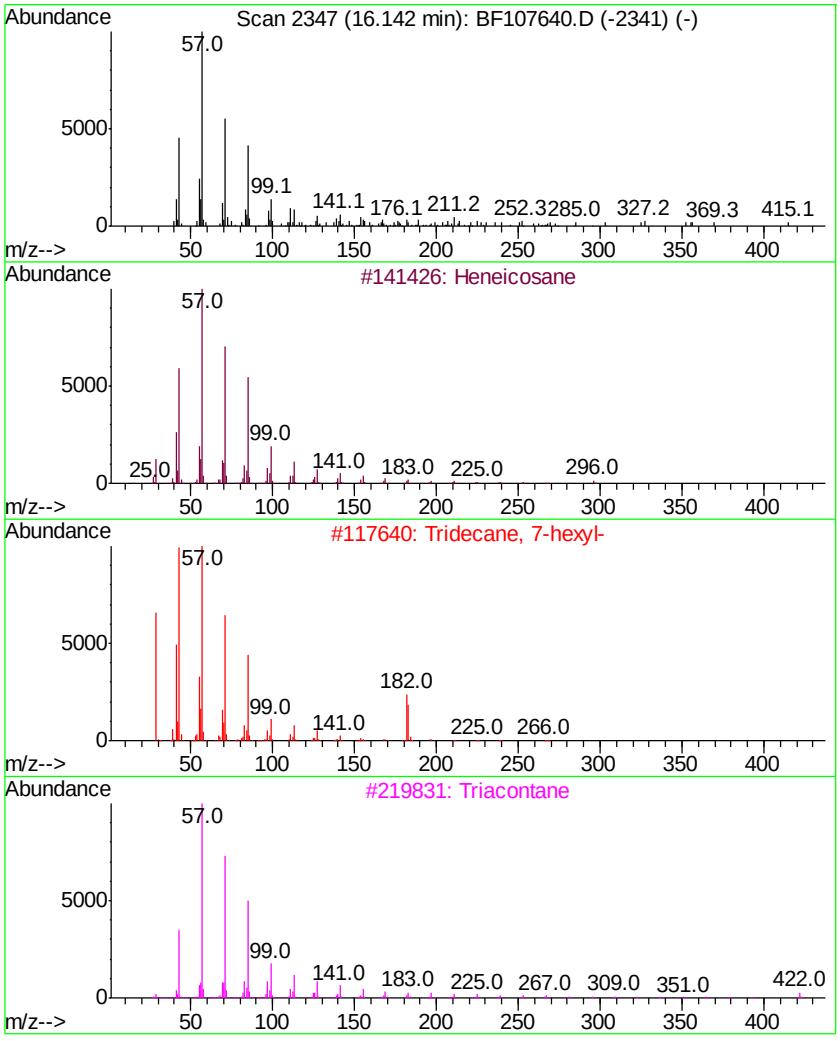
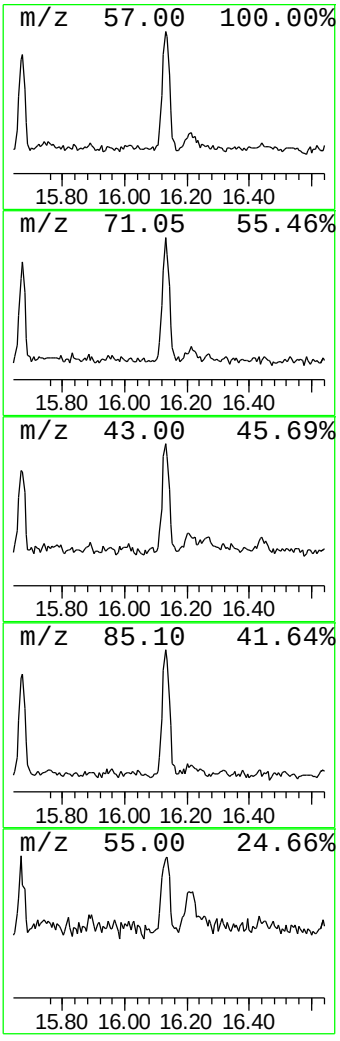
Peak Number 11 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	3.21 ng	205891	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	87
3	Triacontane	422	C30H62	000638-68-6	87
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	86
5	Octadecane	254	C18H38	000593-45-3	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072418\
Data File : BF107640.D
Acq On : 25 Jul 2018 2:38
Operator : JU/SJ
Sample : J4120-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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
2-Pentanone, 4-hy...	5.22	15.6	ng	1335290	1	6.97	1714770	20.0
unknown6.75	6.75	86.7	ng	7428860	1	6.97	1714770	20.0
Anthracene, 2-met...	12.01	2.5	ng	218912	4	11.50	1768050	20.0
Pentafluoropropio...	13.97	9.7	ng	764677	5	14.15	1581580	20.0
Pentacosane	14.28	2.3	ng	184232	5	14.15	1581580	20.0
Hexadecane	14.59	2.4	ng	191375	5	14.15	1581580	20.0
Heptadecane	14.91	3.0	ng	239884	5	14.15	1581580	20.0
Heptadecane, 9-oc...	15.27	2.9	ng	186030	6	15.69	1282040	20.0
Heneicosane	16.14	3.2	ng	205891	6	15.69	1282040	20.0