LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114402.D
Acq On : 18 May 2019 20:09
Operator : JU/SJ
Sample : K2881-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-047

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-BF051019.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	2.151	3	11	22	rVB	1418046	2031224	28.23%	3.066%
2	3.928	308	313	325	rVB	242509	352025	4.89%	0.531%
3	5.475	572	576	600	rBV	6011364	6697232	93.07%	10.108%
4	6.487	742	748	758	rBV	6029448	7195694	100.00%	10.860%
5	6.616	765	770	773	rBV	6528712	6683399	92.88%	10.087%
6	6.834	804	807	816	rBV	1909704	1630339	22.66%	2.461%
7	6.992	830	834	847	rVB	5543632	5159399	71.70%	7.787%
8	7.398	898	903	915	rBV	4080150	4621866	64.23%	6.976%
9	8.116	1021	1025	1042	rBV	2138669	2065094	28.70%	3.117%
10	9.186	1202	1207	1211	rBV	6440673	6911091	96.04%	10.431%
11	9.580	1270	1274	1279	rBV	875151	814894	11.32%	1.230%
12	9.869	1318	1323	1334	rVB	2398645	2261183	31.42%	3.413%
13	10.657	1453	1457	1470	rBV	3988932	4512959	62.72%	6.811%
14	11.351	1571	1575	1589	rBV	2424496	2392857	33.25%	3.612%
15	11.874	1660	1664	1677	rBV	894968	967840	13.45%	1.461%
16	12.574	1778	1783	1791	rBV9	27595	80087	1.11%	0.121%
17	12.657	1794	1797	1805	rBV	197223	246463	3.43%	0.372%
18	12.933	1839	1844	1848	rBV	5609796	5752262	79.94%	8.682%
19	13.157	1876	1882	1885	rBV3	46825	79758	1.11%	0.120%
20	13.498	1935	1940	1943	rBV3	54870	81518	1.13%	0.123%
21	13.821	1991	1995	2006	rBV	846713	1223700	17.01%	1.847%
22	13.992	2020	2024	2031	rBV	1516851	1473843	20.48%	2.224%
23	14.139	2046	2049	2054	rBV2	92190	114967	1.60%	0.174%
24	14.445	2097	2101	2108	rBV	183295	273715	3.80%	0.413%
25	14.745	2149	2152	2157	rVB	133574	139338	1.94%	0.210%
26	14.821	2162	2165	2169	rVB	93971	89757	1.25%	0.135%
27	15.074	2205	2208	2214	rVB	304656	349040	4.85%	0.527%
28	15.457	2268	2273	2284	rBV	1158255	1654206	22.99%	2.497%
29	15.880	2340	2345	2350	rVB	189403	272438	3.79%	0.411%
30	15.945	2352	2356	2362	rBV5	55258	128397	1.78%	0.194%

Sum of corrected areas: 66256585

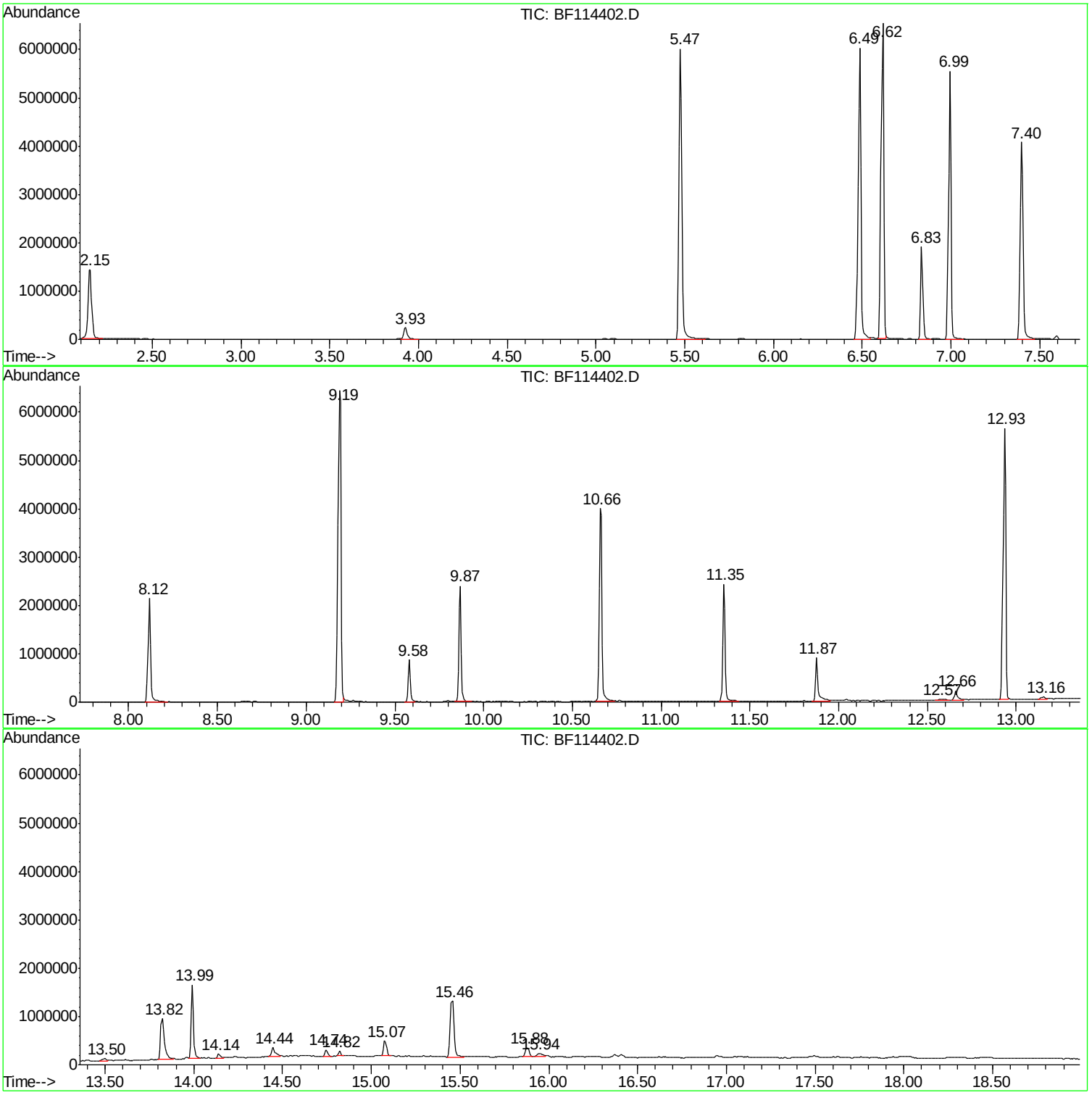
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114402.D
Acq On : 18 May 2019 20:09
Operator : JU/SJ
Sample : K2881-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-047

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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Data File : BF114402.D
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

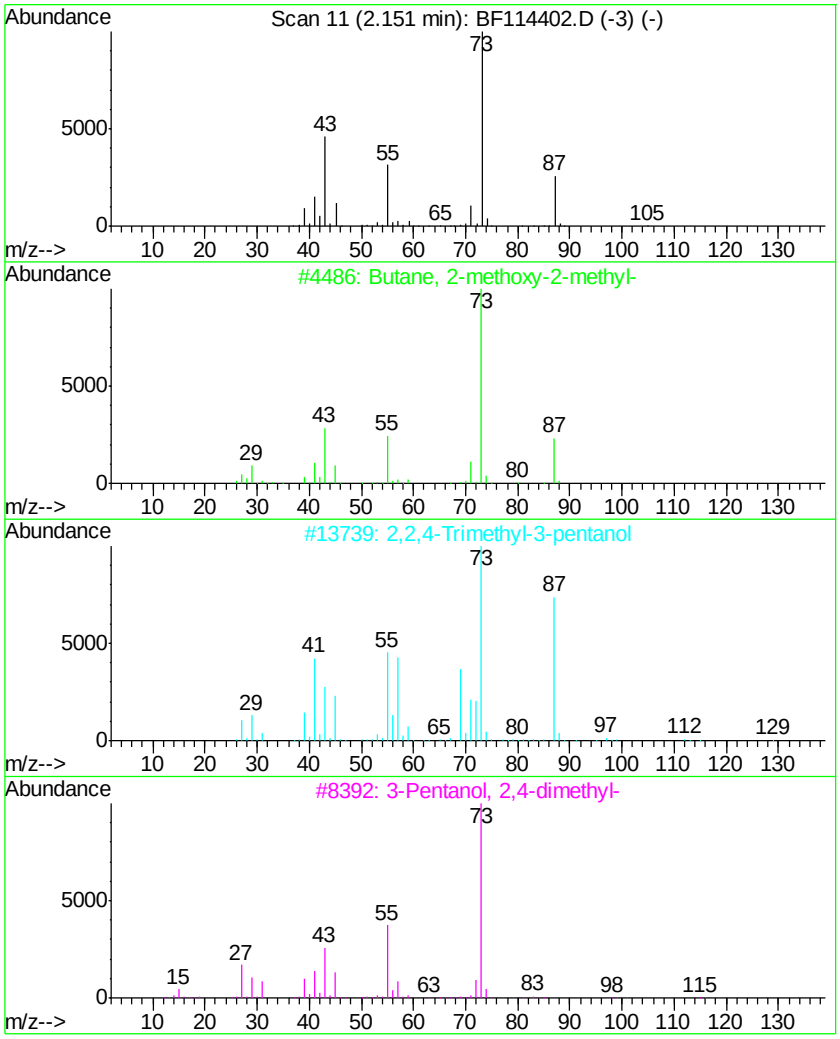
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

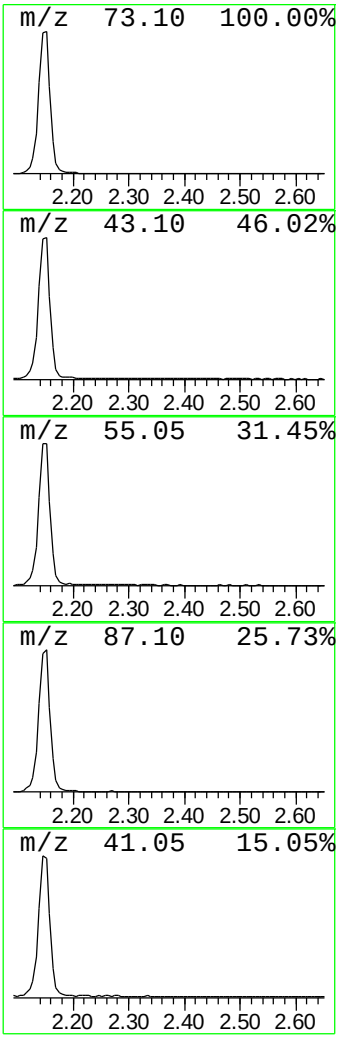
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	24.92 ng	2031220	1,4-Dichlorobenzene-d4	6.83

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	39
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Misc :
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Instrument : BNA_F
ClientSampleId : FK-PS-01-047

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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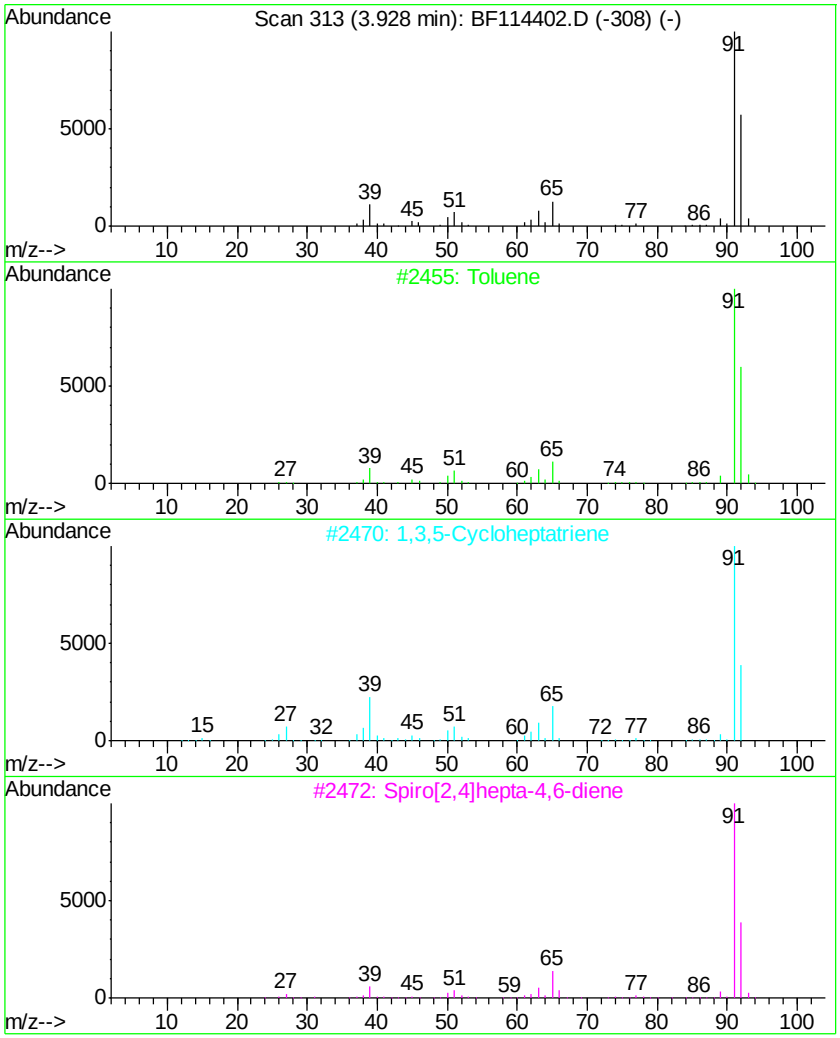
TIC Integration Parameters: LSCINT.P

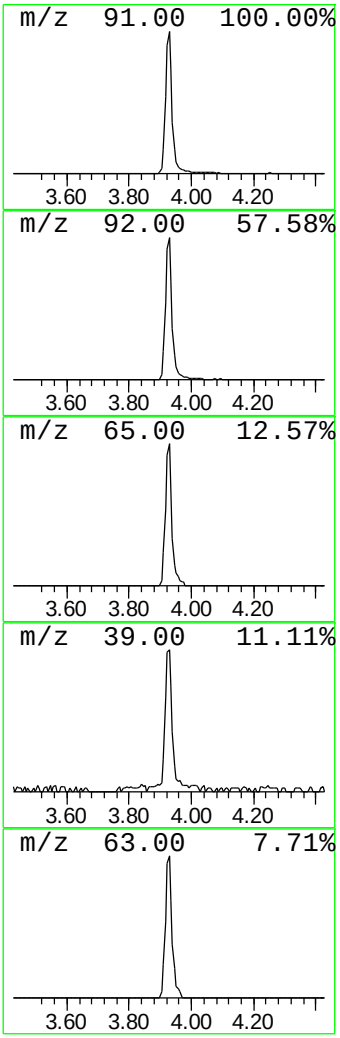
****

Peak Number 2 1,3,5-Cycloheptatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.93	4.32 ng	352025	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	95
2	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	90
3	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	87
4	2,5-Norbornadiene	92	C7H8	000121-46-0	83
5	Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	72





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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : FK-PS-01-047

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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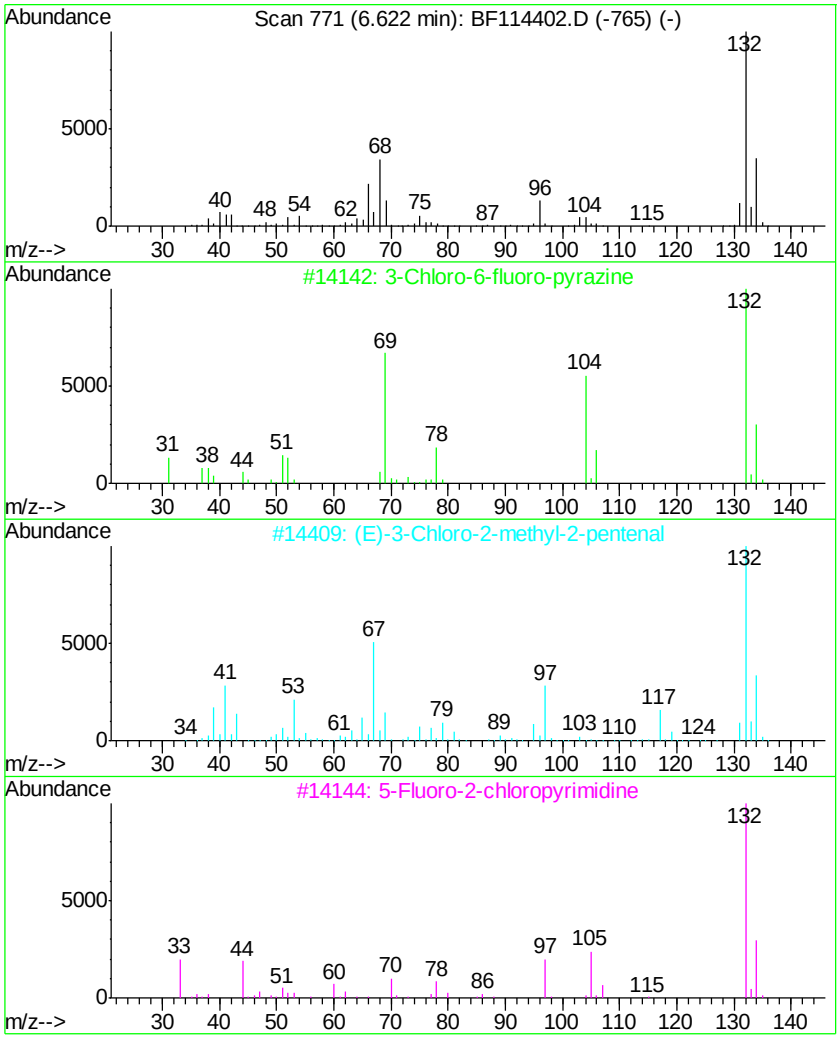
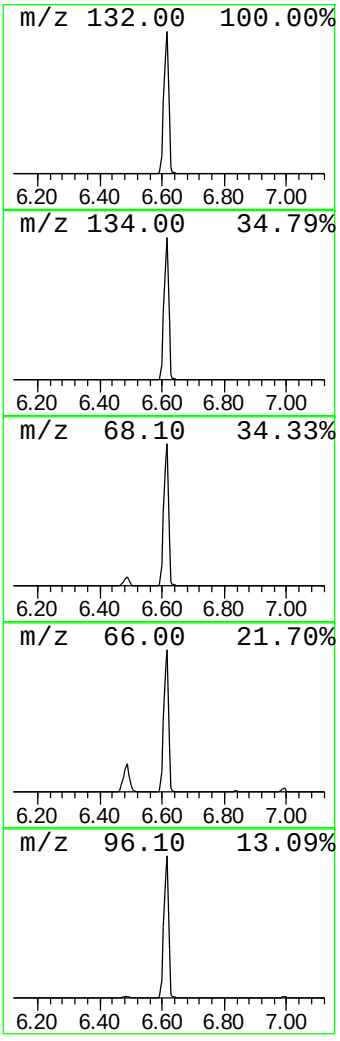
Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	81.99 ng	6683400	1,4-Dichlorobenzene-d4	6.83

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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : FK-PS-01-047

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

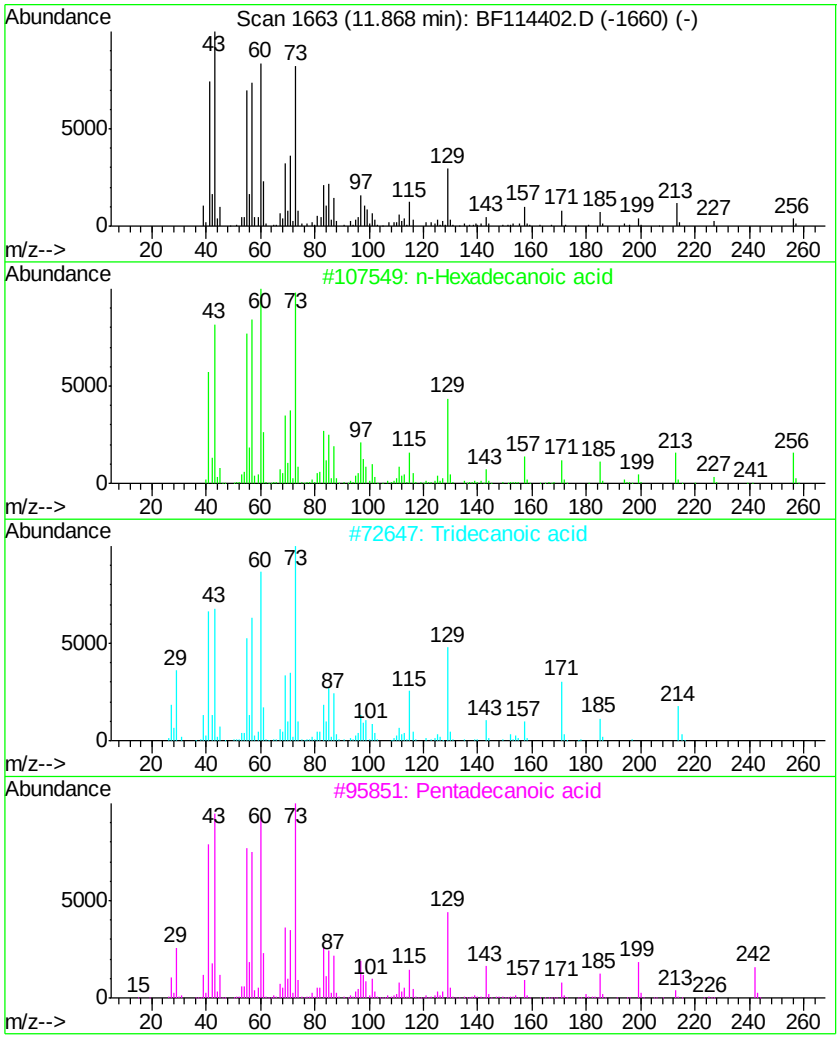
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

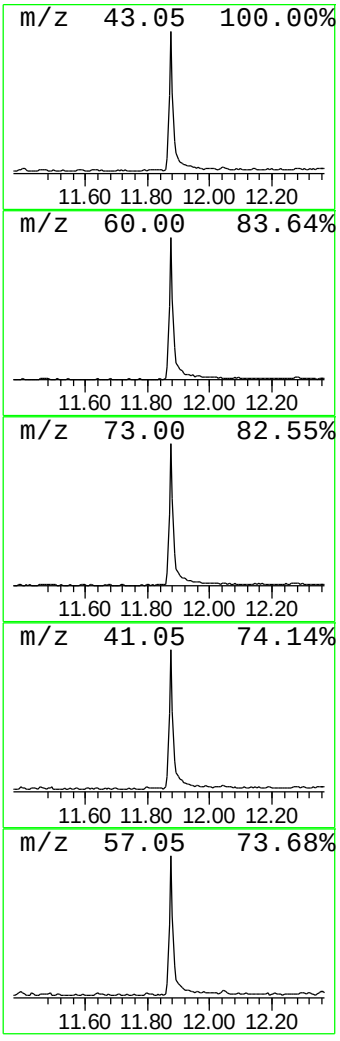
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	8.09 ng	967840	Phenanthrene-d10	11.35

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	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Sample : K2881-01
Misc :
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Instrument : BNA_F
ClientSampleId : FK-PS-01-047

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

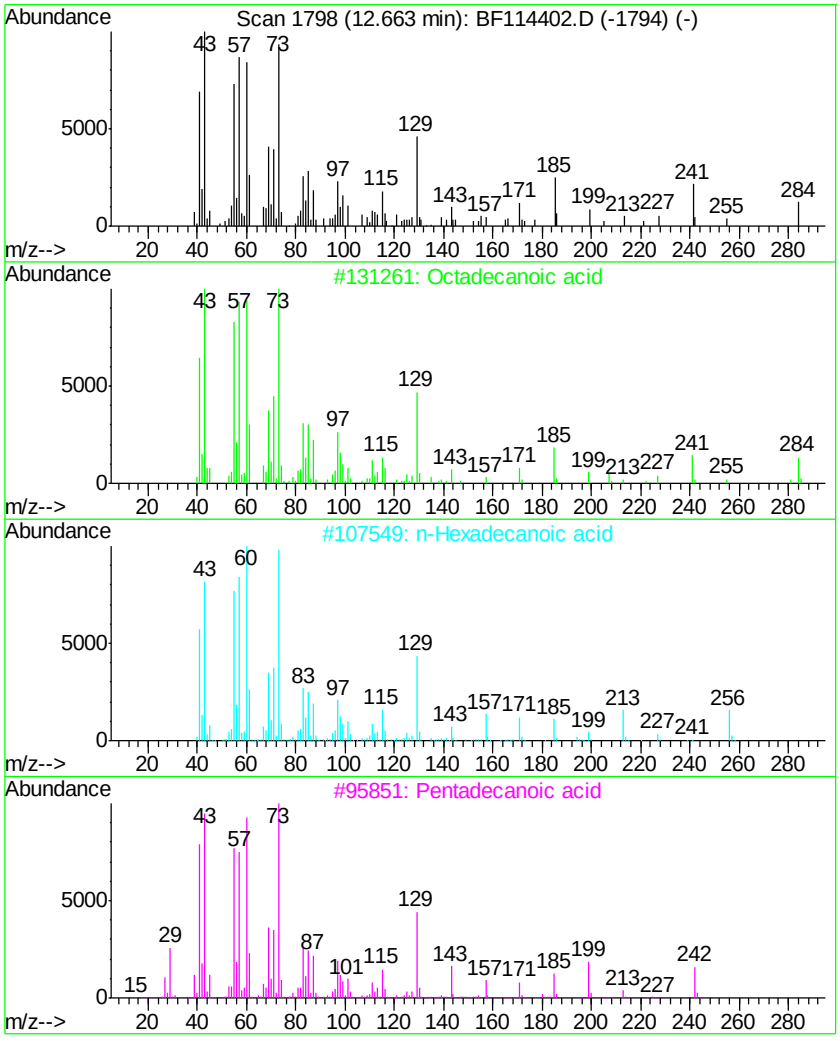
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

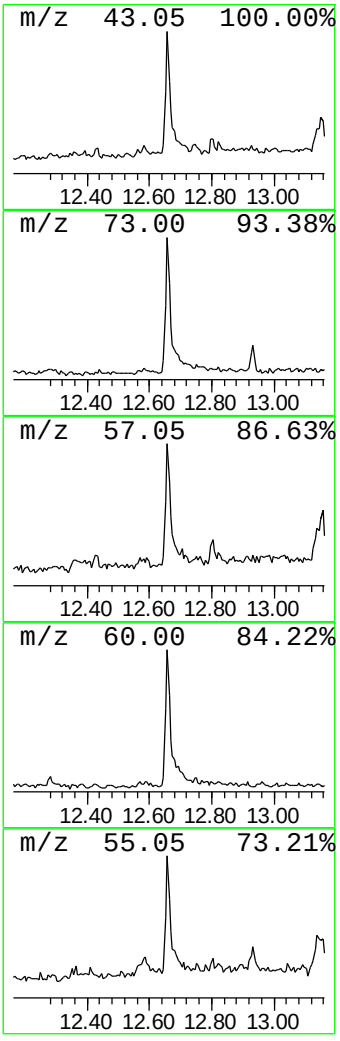
****

Peak Number 6 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	2.06 ng	246463	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : FK-PS-01-047

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
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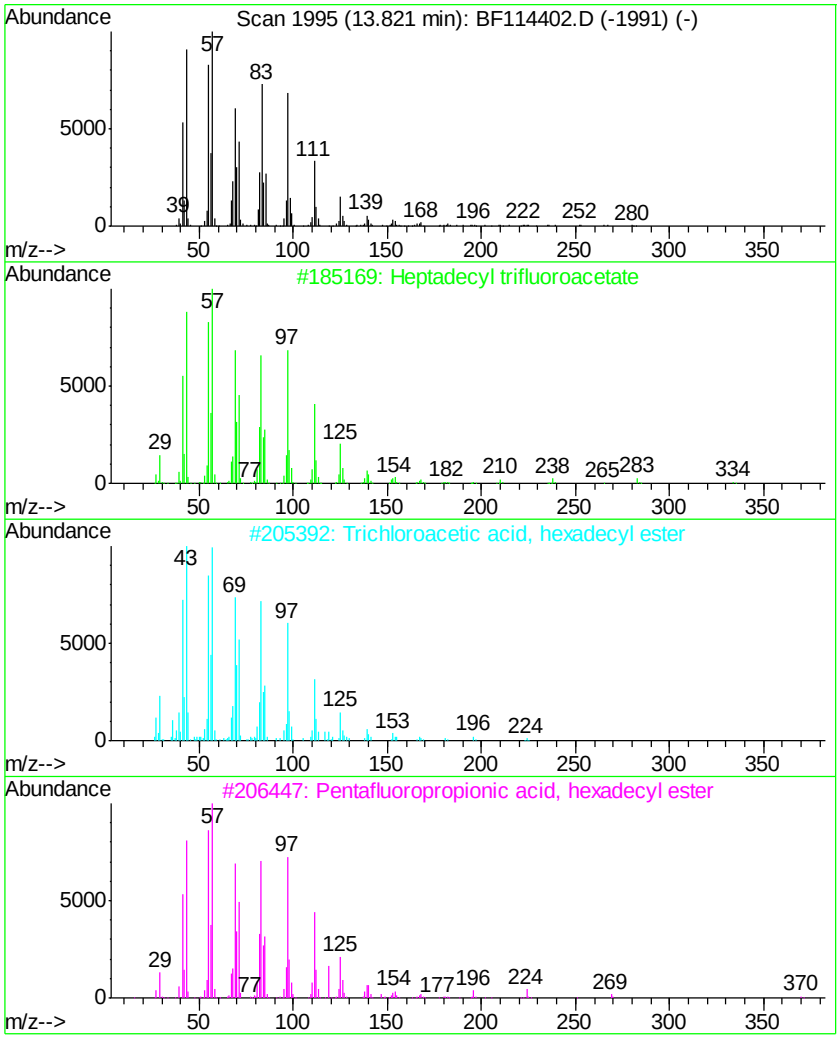
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

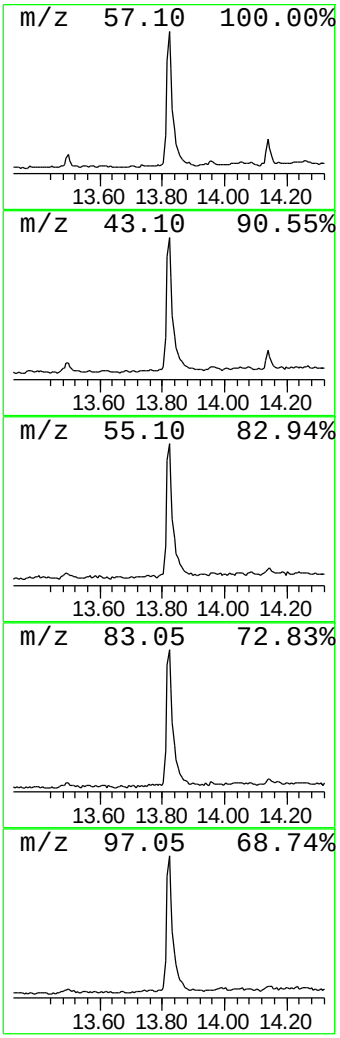
****

Peak Number 7 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	16.61 ng	1223700	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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Misc :
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Instrument :
BNA_F
ClientSampleId :
FK-PS-01-047

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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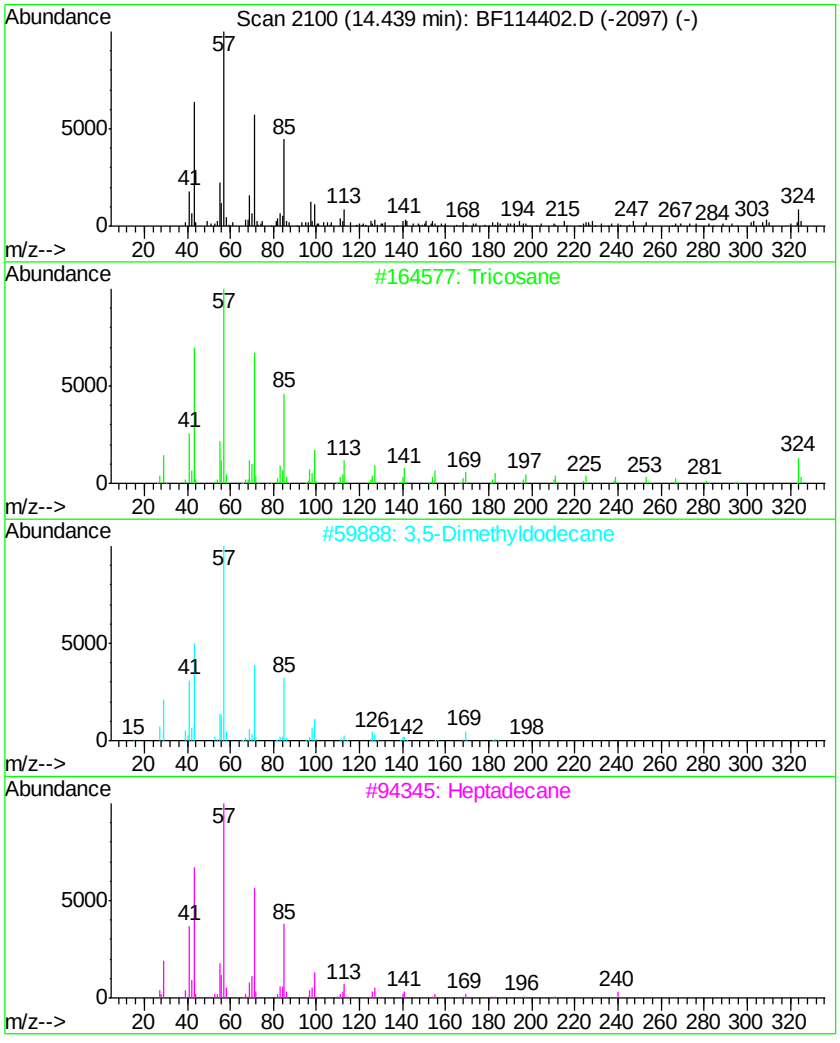
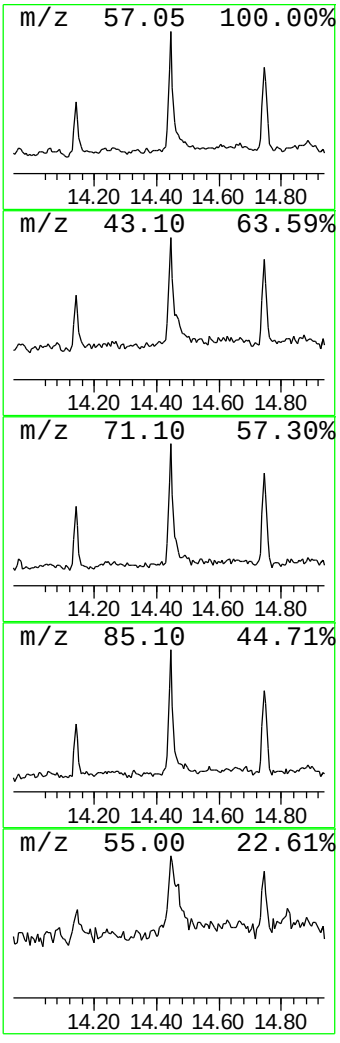
Peak Number 8 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	3.71 ng	273715	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	87
2	3,5-Dimethyldodecane	198	C14H30	107770-99-0	83
3	Heptadecane	240	C17H36	000629-78-7	80
4	Octacosane	394	C28H58	000630-02-4	76
5	Hexadecane	226	C16H34	000544-76-3	72





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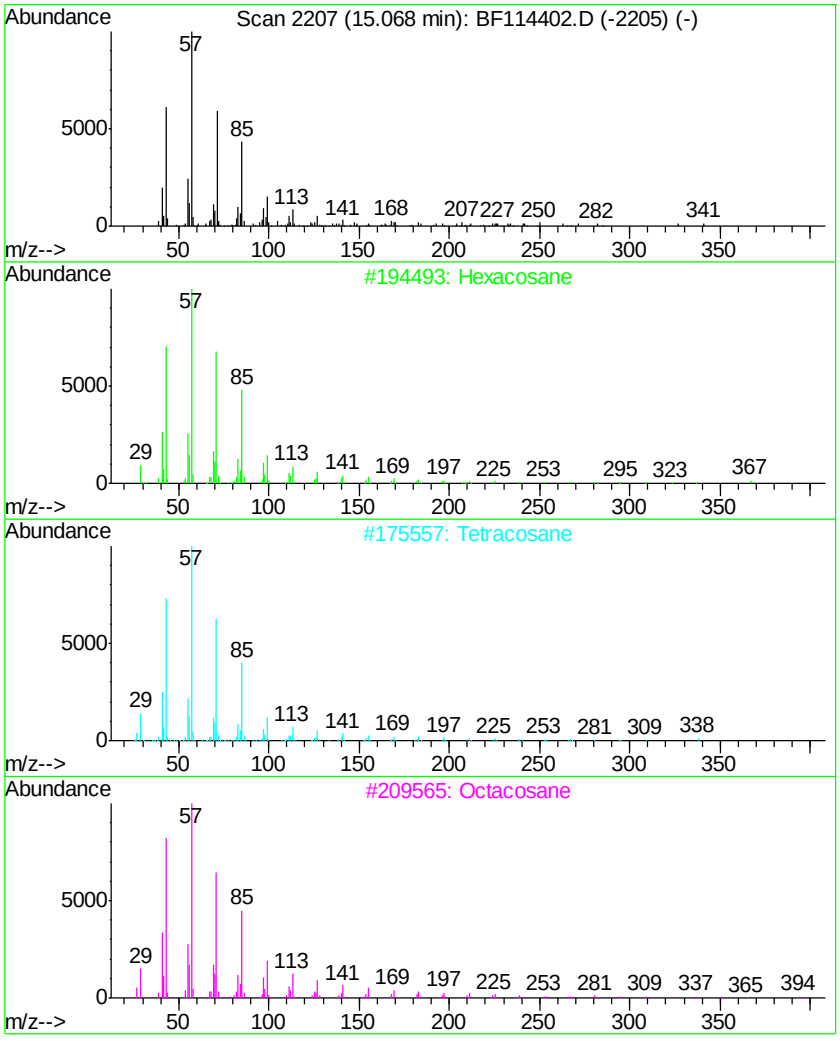
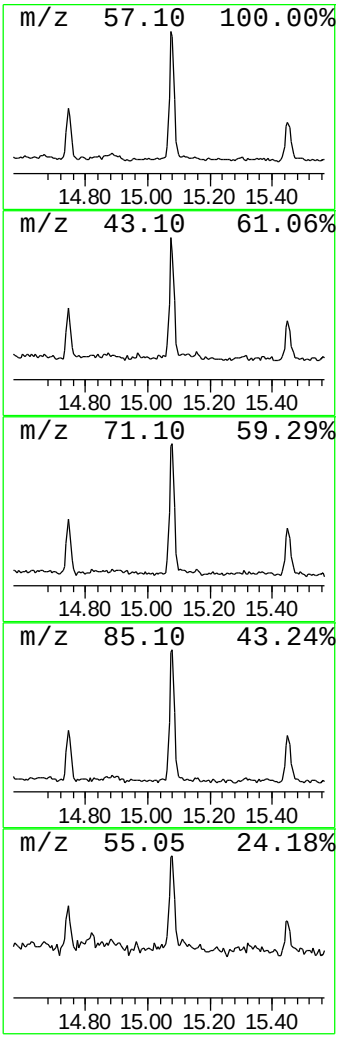
****

Peak Number 9 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	4.22 ng	349040	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Heneicosane	296	C21H44	000629-94-7	90





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Misc :
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Instrument : BNA_F
ClientSampleId : FK-PS-01-047

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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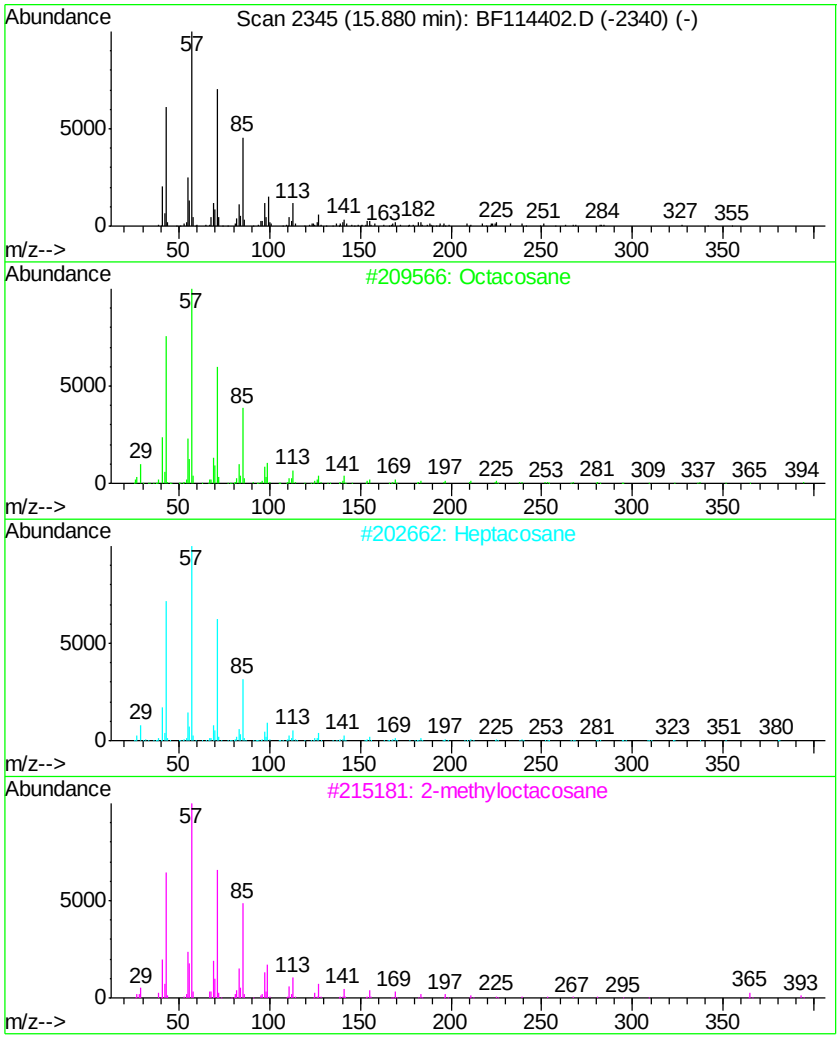
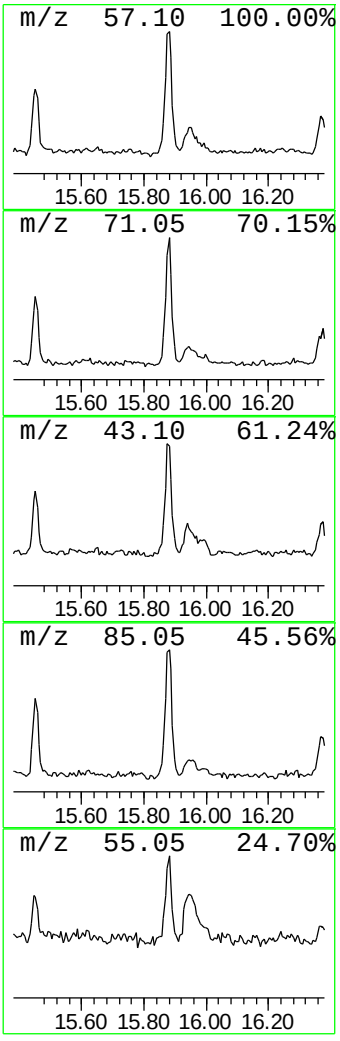
Peak Number 10 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	3.29 ng	272438	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Heptacosane	380	C27H56	000593-49-7	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Hexacosane	366	C26H54	000630-01-3	86
5	Docosane	310	C22H46	000629-97-0	86





Tentatively Identified Compound (LSC) summary

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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...	2.15	24.9	ng	2031220	1	6.83	1630340	20.0
1,3,5-Cycloheptat...	3.93	4.3	ng	352025	1	6.83	1630340	20.0
unknown6.62	6.62	82.0	ng	6683400	1	6.83	1630340	20.0
n-Hexadecanoic acid	11.87	8.1	ng	967840	4	11.35	2392860	20.0
Octadecanoic acid	12.66	2.1	ng	246463	4	11.35	2392860	20.0
Heptadecyl triflu...	13.82	16.6	ng	1223700	5	13.99	1473840	20.0
Tricosane	14.44	3.7	ng	273715	5	13.99	1473840	20.0
Hexacosane	15.07	4.2	ng	349040	6	15.46	1654210	20.0
Octacosane	15.88	3.3	ng	272438	6	15.46	1654210	20.0