LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109389.D
Acq On : 27 Sep 2018 16:12
Operator : JU/SJ
Sample : J5066-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q1-F3

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-BF092218.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	4.898	474	478	486	rVB	51807	67996	3.01%	0.323%
2	5.316	544	549	552	rBV	1895844	1776906	78.77%	8.434%
3	6.345	719	724	729	rBV	2039358	1955913	86.71%	9.283%
4	6.475	742	746	749	rBV	2189935	1920870	85.16%	9.117%
5	6.704	782	785	788	rBV	873090	696299	30.87%	3.305%
6	6.734	788	790	794	rVB	71033	56901	2.52%	0.270%
7	6.775	794	797	800	rBV	24243	28880	1.28%	0.137%
8	6.863	808	812	815	rVB	1805481	1454771	64.49%	6.905%
9	6.986	829	833	838	rVB4	20868	35829	1.59%	0.170%
10	7.263	876	880	884	rVB	1213033	1198203	53.12%	5.687%
11	7.986	999	1003	1006	rBV	1161858	917373	40.67%	4.354%
12	9.063	1182	1186	1189	rBV	2768681	2255719	100.00%	10.706%
13	9.457	1249	1253	1256	rBV	779608	592684	26.27%	2.813%
14	9.739	1297	1301	1304	rBV	1149328	1062027	47.08%	5.041%
15	10.522	1430	1434	1444	rBV	1487147	1324860	58.73%	6.288%
16	11.216	1548	1552	1554	rBV	1207489	1080519	47.90%	5.129%
17	11.233	1554	1555	1559	rVB	111846	72151	3.20%	0.342%
18	11.745	1639	1642	1646	rBV2	35401	46711	2.07%	0.222%
19	12.416	1753	1756	1760	rVB	132483	121251	5.38%	0.575%
20	12.645	1789	1795	1798	rBV	126709	127849	5.67%	0.607%
21	12.798	1816	1821	1824	rVB	2035818	1877243	83.22%	8.910%
22	13.710	1973	1976	1987	rVB4	59737	99796	4.42%	0.474%
23	13.839	1993	1998	2001	rBV	909256	830404	36.81%	3.941%
24	14.321	2078	2080	2083	rBV	32654	31493	1.40%	0.149%
25	14.592	2123	2126	2128	rBV2	24803	26739	1.19%	0.127%
26	14.621	2128	2131	2136	rVB	58635	61814	2.74%	0.293%
27	14.845	2165	2169	2172	rBV2	47263	70546	3.13%	0.335%
28	14.933	2180	2184	2189	rVB2	67741	78503	3.48%	0.373%
29	15.121	2213	2216	2221	rVV	31742	35799	1.59%	0.170%
30	15.180	2222	2226	2231	rVB	39565	47647	2.11%	0.226%
31	15.239	2231	2236	2240	rBV	653096	759812	33.68%	3.606%
32	15.286	2241	2244	2248	rVB	81751	95611	4.24%	0.454%
33	15.686	2307	2312	2317	rBV	80637	107381	4.76%	0.510%
34	16.151	2386	2391	2396	rBV	49729	77329	3.43%	0.367%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109389.D
Acq On : 27 Sep 2018 16:12
Operator : JU/SJ
Sample : J5066-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q1-F3

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-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.586	2461	2465	2469	rVB2	18071	28482	1.26%	0.135%
36	16.686	2478	2482	2489	rVB3	24844	46573	2.06%	0.221%

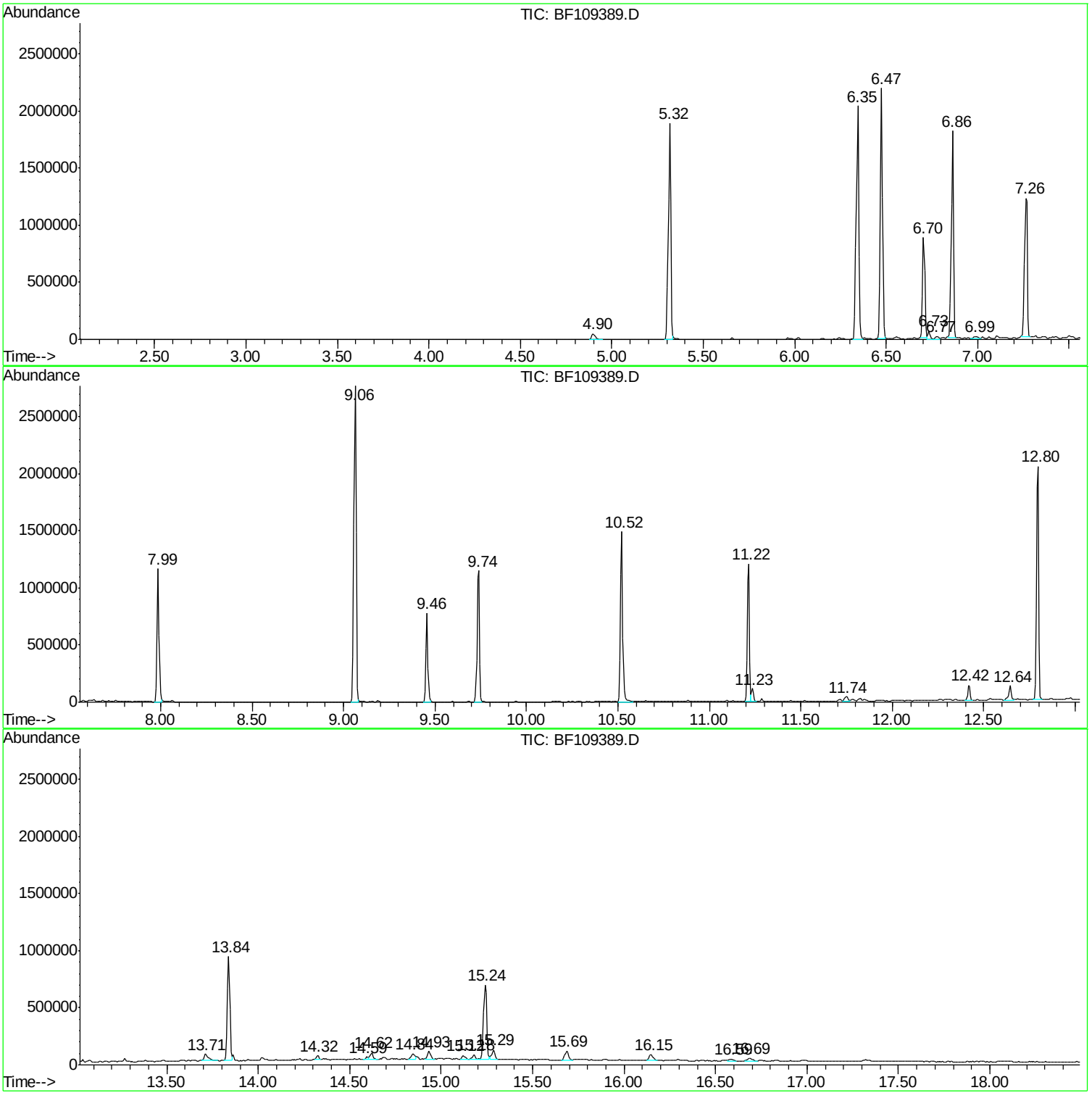
Sum of corrected areas: 21068884

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109389.D
Acq On : 27 Sep 2018 16:12
Operator : JU/SJ
Sample : J5066-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q1-F3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109389.D
Acq On : 27 Sep 2018 16:12
Operator : JU/SJ
Sample : J5066-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q1-F3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

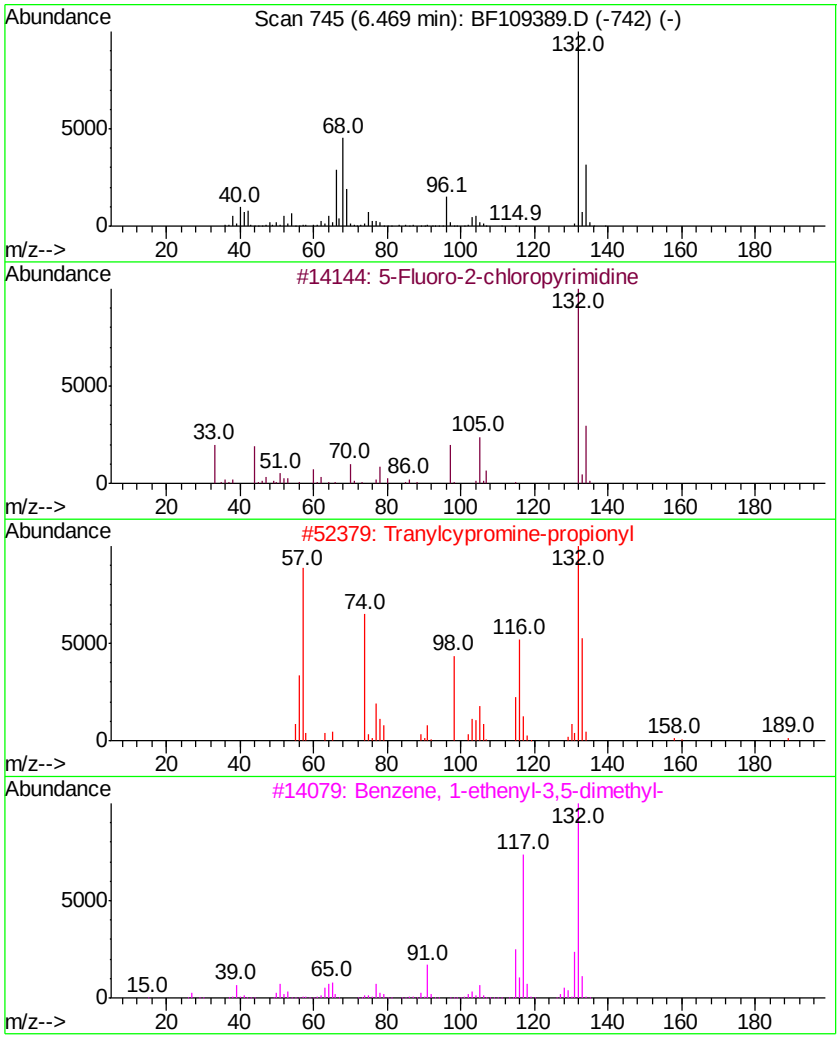
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

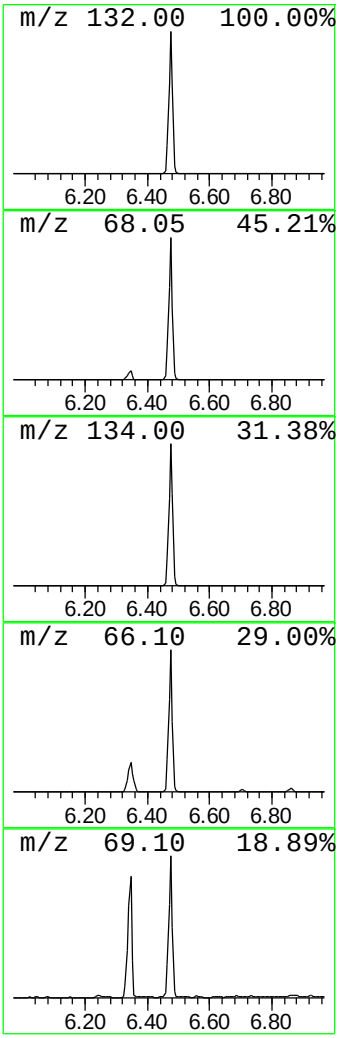
****

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	55.17 ng	1920870	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109389.D
Acq On : 27 Sep 2018 16:12
Operator : JU/SJ
Sample : J5066-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q1-F3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

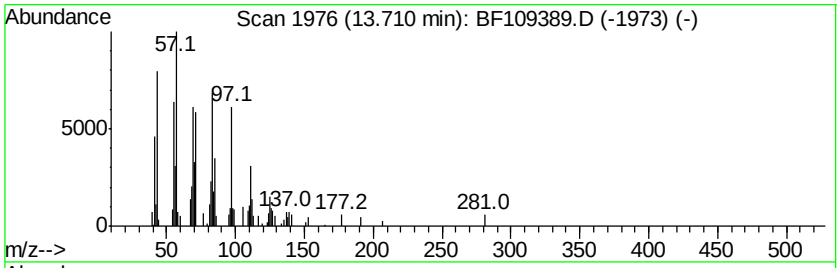
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

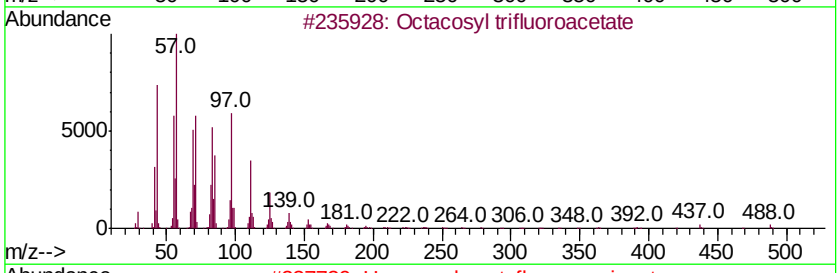
****

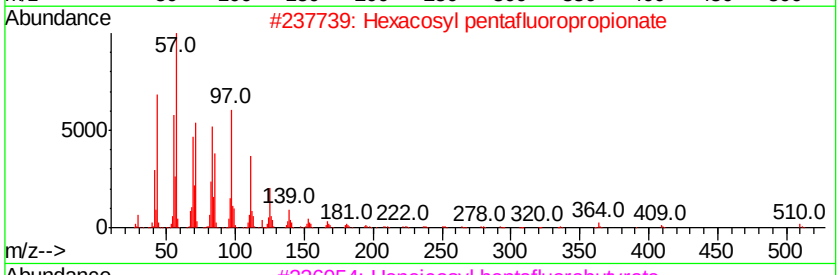
Peak Number 3 Octacosyl trifluoroacetate Concentration Rank 4

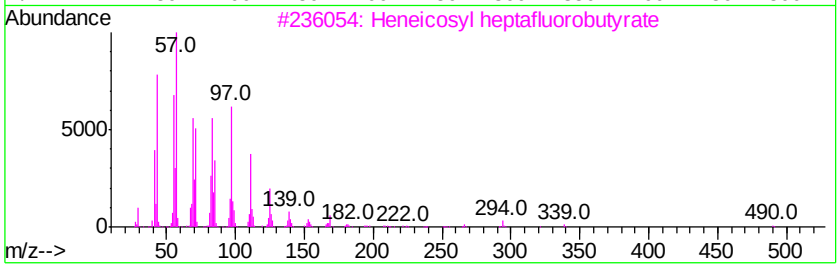
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	2.40 ng	99796	Chrysene-d12	13.84

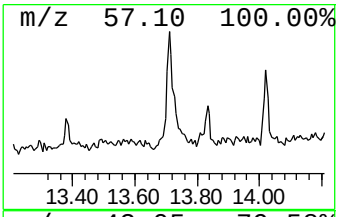
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	87
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87
4	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	86
5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	86

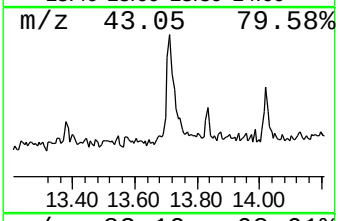


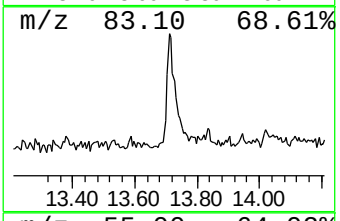


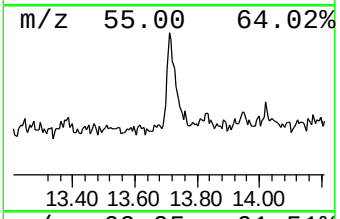


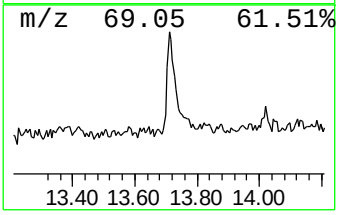












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109389.D
Acq On : 27 Sep 2018 16:12
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Sample : J5066-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q1-F3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

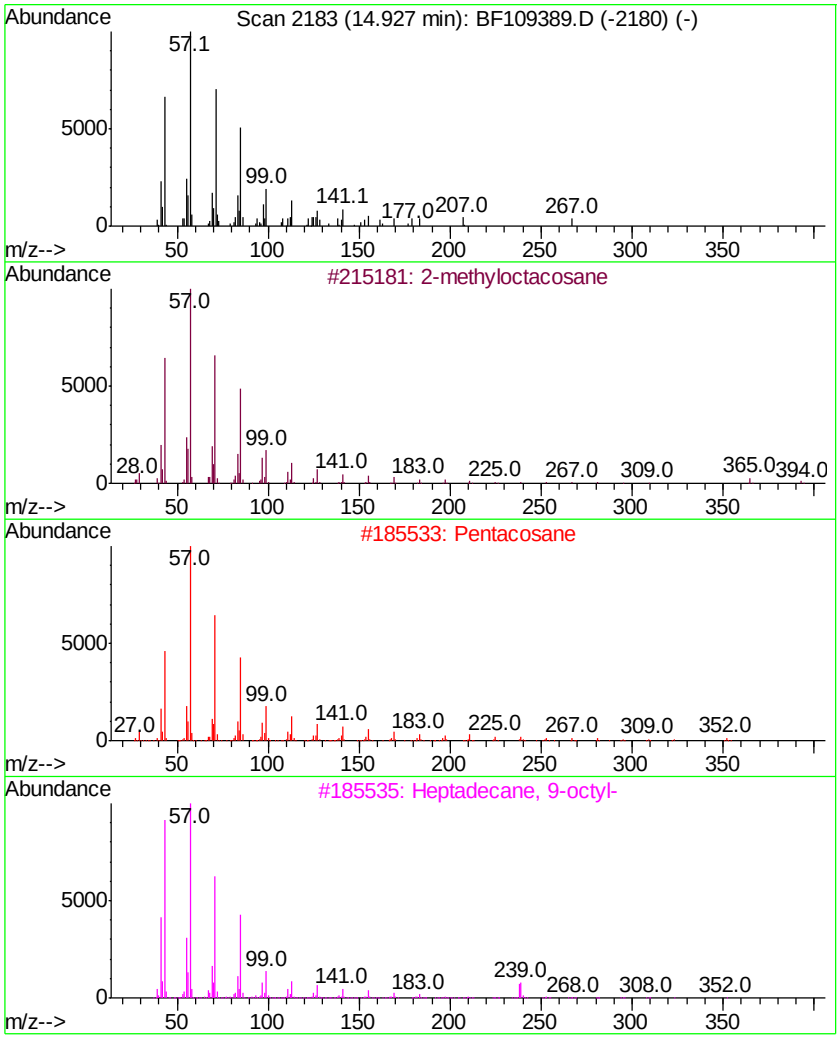
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

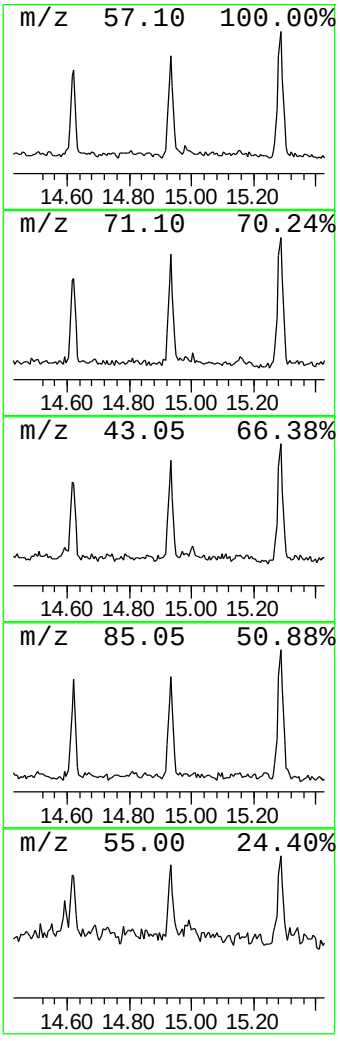
****

Peak Number 4 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.07 ng	78503	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Pentacosane	352	C25H52	000629-99-2	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109389.D
Acq On : 27 Sep 2018 16:12
Operator : JU/SJ
Sample : J5066-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q1-F3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

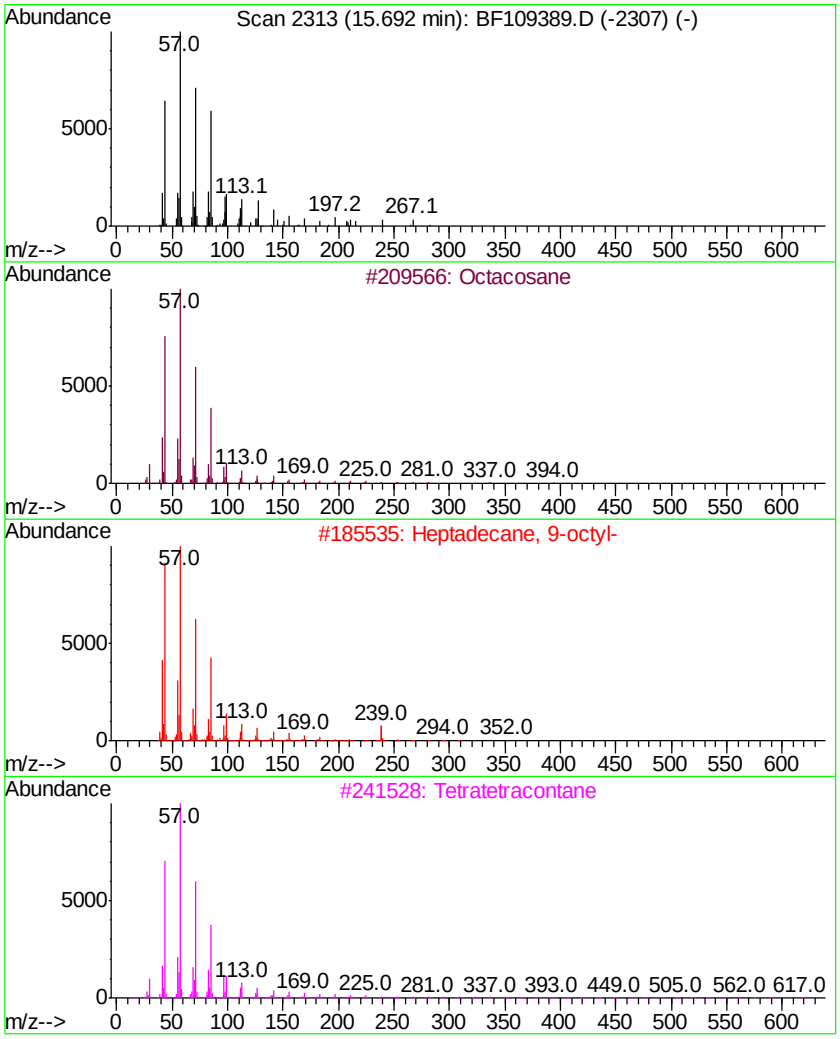
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

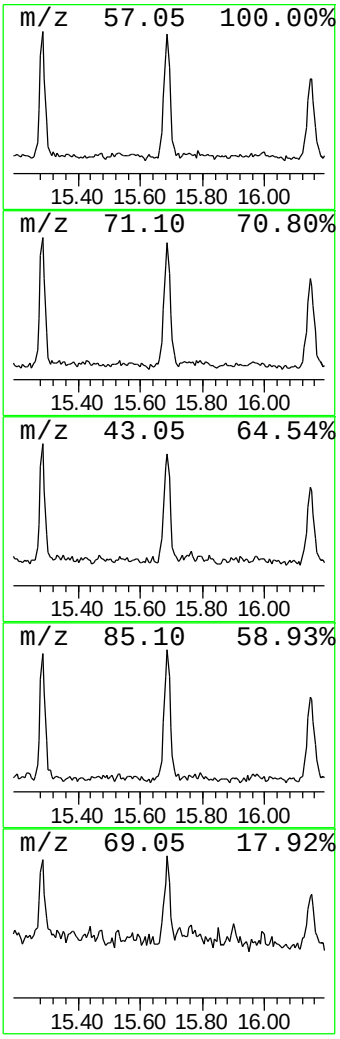
****

Peak Number 5 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	2.83 ng	107381	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Triacontane	422	C30H62	000638-68-6	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109389.D
Acq On : 27 Sep 2018 16:12
Operator : JU/SJ
Sample : J5066-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q1-F3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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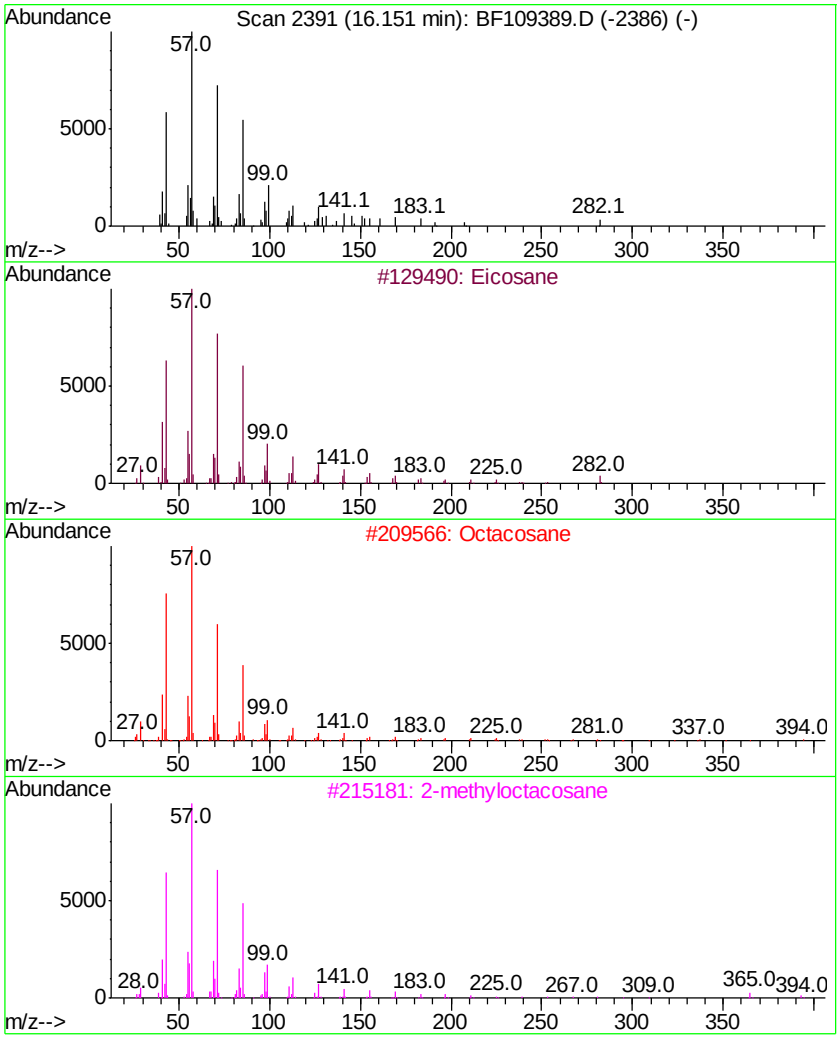
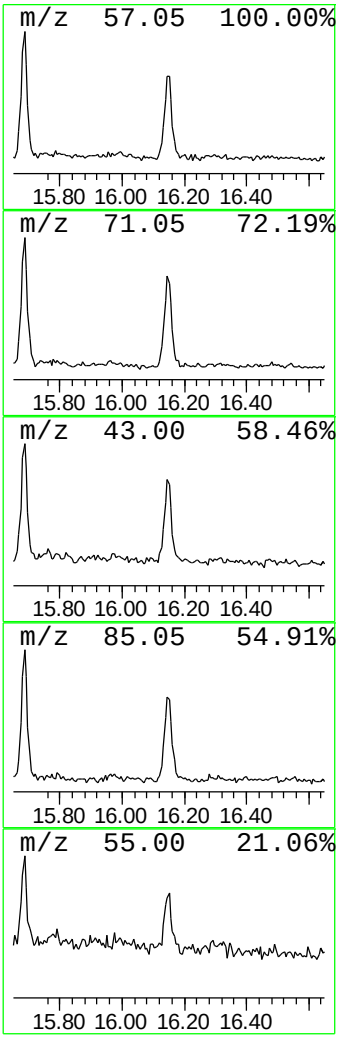
Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	2.04 ng	77329	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Octacosane	394	C28H58	000630-02-4	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109389.D
Acq On : 27 Sep 2018 16:12
Operator : JU/SJ
Sample : J5066-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q1-F3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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
unknown6.47	6.47	55.2	ng	1920870	1	6.70	696299	20.0
Octacosyl trifluo...	13.71	2.4	ng	99796	5	13.84	830404	20.0
2-methyloctacosane	14.93	2.1	ng	78503	6	15.24	759812	20.0
Octacosane	15.69	2.8	ng	107381	6	15.24	759812	20.0
Eicosane	16.15	2.0	ng	77329	6	15.24	759812	20.0