LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121937.D
Acq On : 13 Oct 2020 14:35
Operator : JU/CG
Sample : L4369-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-3

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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF121937.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	484	489	500	rBV	39769	61804	1.96%	0.241%
2	5.369	554	558	575	rBV	2741235	2759236	87.69%	10.778%
3	6.387	727	731	748	rBV	2578166	2862568	90.97%	11.182%
4	6.587	761	765	776	rBV3	17658	43121	1.37%	0.168%
5	6.740	788	791	798	rBV	890941	746995	23.74%	2.918%
6	7.310	883	888	891	rBV	2052685	1916694	60.91%	7.487%
7	8.022	1005	1009	1018	rBV	1047834	997532	31.70%	3.897%
8	9.098	1187	1192	1196	rBV	3143603	3146574	100.00%	12.291%
9	9.498	1255	1260	1267	rVB	281776	277926	8.83%	1.086%
10	9.775	1302	1307	1311	rBV	1266878	1098374	34.91%	4.290%
11	10.569	1437	1442	1445	rBV	2066085	1982119	62.99%	7.743%
12	11.263	1555	1560	1562	rBV	1158907	1104947	35.12%	4.316%
13	11.280	1562	1563	1567	rVB	163065	128853	4.10%	0.503%
14	11.422	1584	1587	1592	rVB	34172	36278	1.15%	0.142%
15	11.763	1641	1645	1647	rBV	51421	53342	1.70%	0.208%
16	11.792	1647	1650	1657	rVV2	194810	205279	6.52%	0.802%
17	11.869	1660	1663	1666	rBV	50197	52322	1.66%	0.204%
18	11.898	1666	1668	1672	rVB2	31885	39461	1.25%	0.154%
19	11.939	1672	1675	1677	rBV3	26283	32280	1.03%	0.126%
20	12.310	1735	1738	1741	rBV	43170	37913	1.20%	0.148%
21	12.475	1762	1766	1770	rVB	277840	258392	8.21%	1.009%
22	12.610	1786	1789	1793	rBV4	30288	48951	1.56%	0.191%
23	12.698	1799	1804	1810	rBV	259082	280567	8.92%	1.096%
24	12.845	1825	1829	1833	rBV	2969252	2787667	88.59%	10.889%
25	12.922	1839	1842	1847	rVB4	24648	37897	1.20%	0.148%
26	13.027	1858	1860	1863	rVB	43613	48261	1.53%	0.189%
27	13.074	1865	1868	1870	rBV	40798	42451	1.35%	0.166%
28	13.133	1876	1878	1882	rVB2	41460	37406	1.19%	0.146%
29	13.416	1922	1926	1931	rBV5	25916	51346	1.63%	0.201%
30	13.751	1979	1983	1993	rVB	372106	620062	19.71%	2.422%
31	13.898	2001	2008	2011	rBV	953010	1026319	32.62%	4.009%
32	13.927	2011	2013	2021	rVB	127069	122320	3.89%	0.478%
33	14.063	2032	2036	2038	rBV	66590	84866	2.70%	0.332%
34	14.363	2083	2087	2089	rBV	97369	97772	3.11%	0.382%
35	14.398	2089	2093	2105	rVB4	63238	148772	4.73%	0.581%
36	14.663	2134	2138	2141	rVB	104458	112854	3.59%	0.441%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121937.D
Acq On : 13 Oct 2020 14:35
Operator : JU/CG
Sample : L4369-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-3

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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.733	2147	2150	2154	rVB	44642	41857	1.33%	0.164%
38	14.927	2179	2183	2189	rBV	108338	199696	6.35%	0.780%
39	14.986	2189	2193	2197	rVB	162347	194776	6.19%	0.761%
40	15.033	2198	2201	2205	rBV4	39153	61080	1.94%	0.239%
41	15.216	2228	2232	2239	rVB	76034	109407	3.48%	0.427%
42	15.274	2239	2242	2247	rVB	91378	113122	3.60%	0.442%
43	15.333	2248	2252	2263	rVB2	665324	966313	30.71%	3.775%
44	15.757	2319	2324	2330	rVB	122841	181927	5.78%	0.711%
45	15.839	2334	2338	2341	rBV5	53381	95267	3.03%	0.372%
46	16.233	2400	2405	2408	rBV	55220	90273	2.87%	0.353%
47	16.739	2488	2491	2496	rBV2	36736	66681	2.12%	0.260%
48	17.168	2559	2564	2574	rVB	39204	90465	2.88%	0.353%

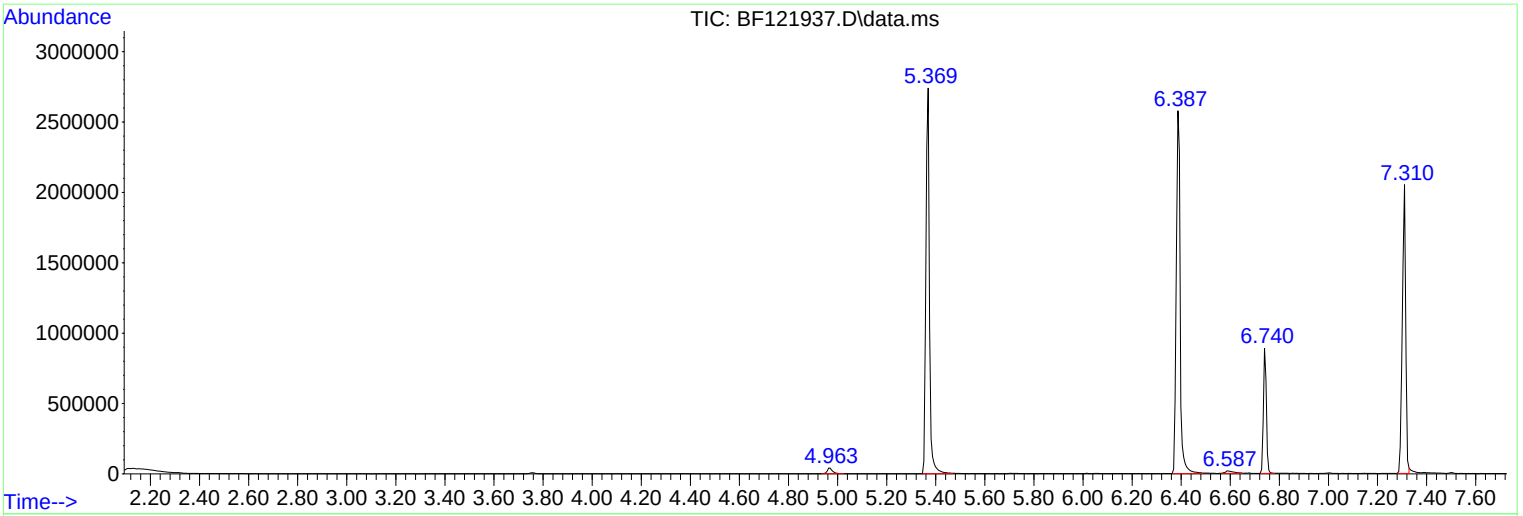
Sum of corrected areas: 25600385

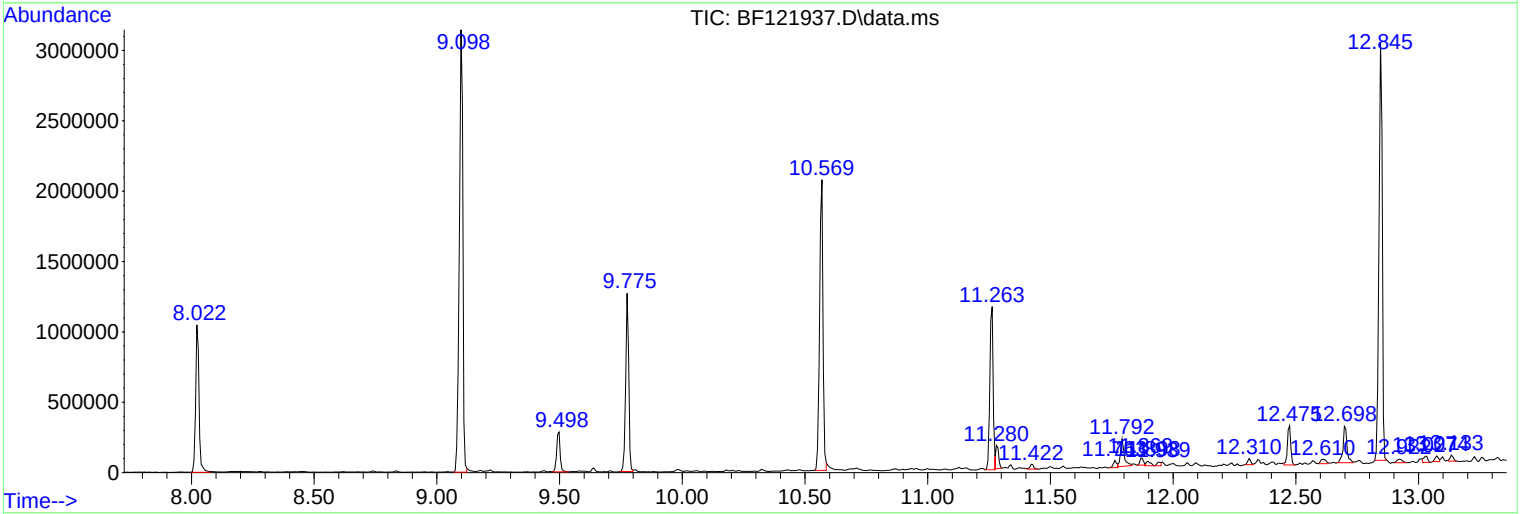
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121937.D
Acq On : 13 Oct 2020 14:35
Operator : JU/CG
Sample : L4369-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

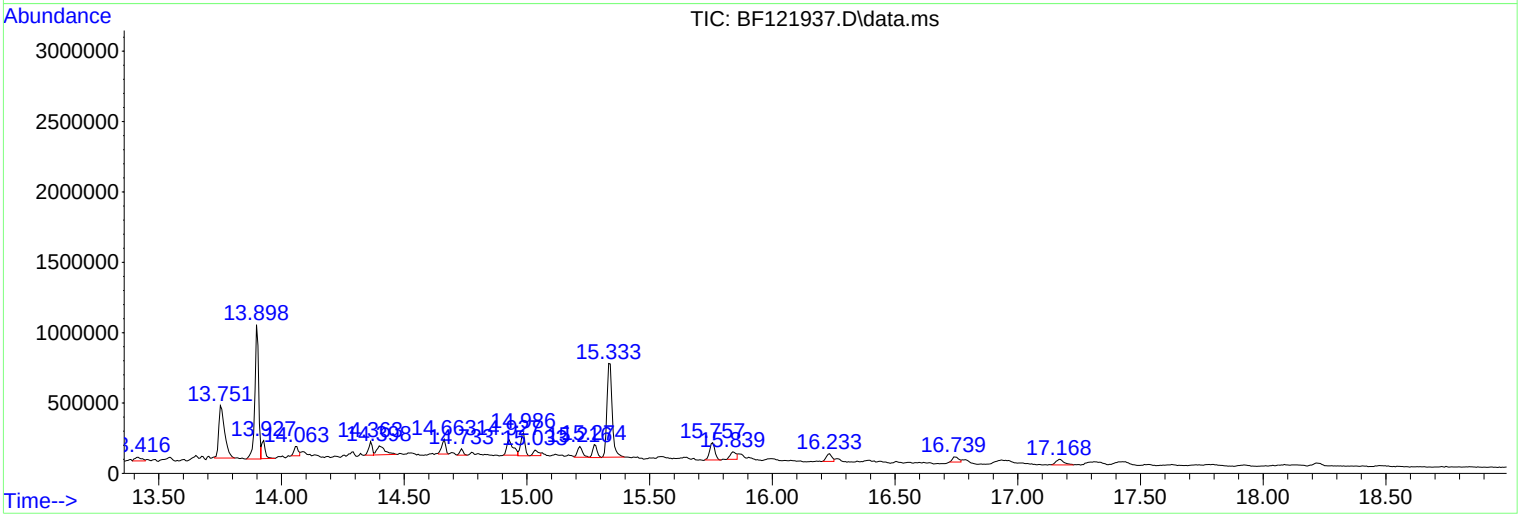
Instrument :
BNA_F
ClientSampleId :
HD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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\BF101320\
Data File : BF121937.D
Acq On : 13 Oct 2020 14:35
Operator : JU/CG
Sample : L4369-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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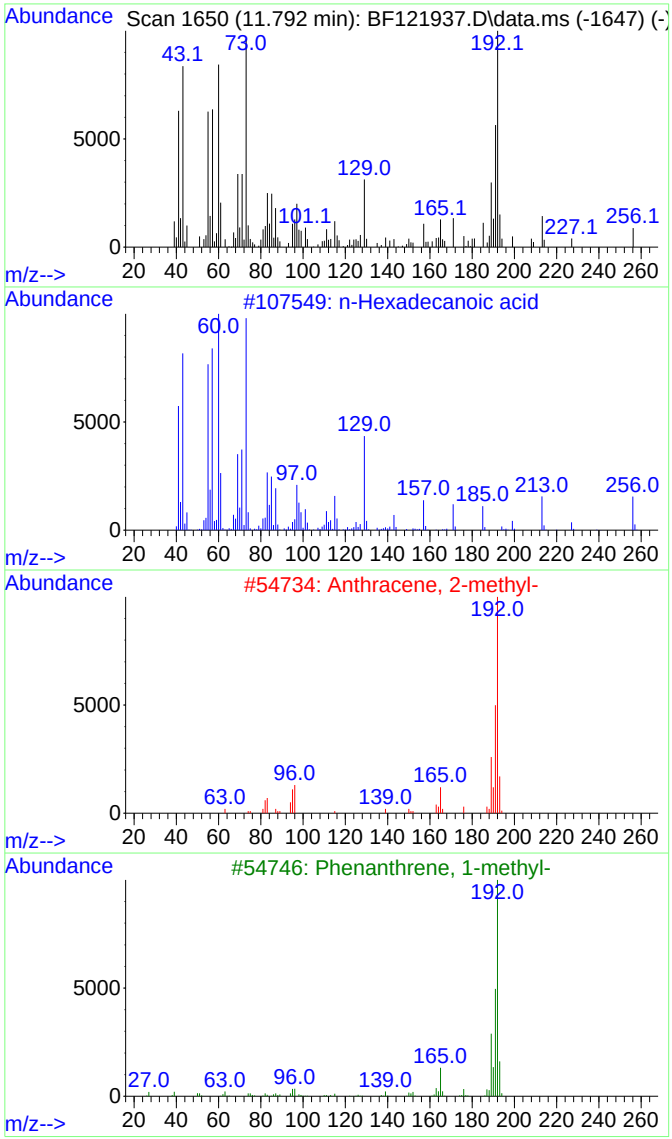
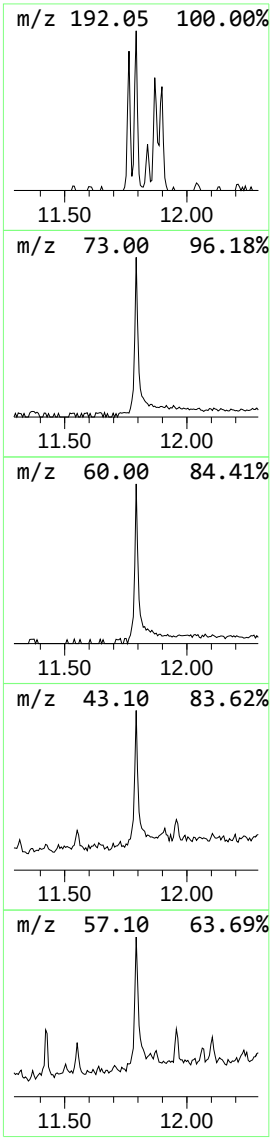
Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	3.72 ng	205279	Phenanthrene-d10	11.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	74
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	74
5	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121937.D
Acq On : 13 Oct 2020 14:35
Operator : JU/CG
Sample : L4369-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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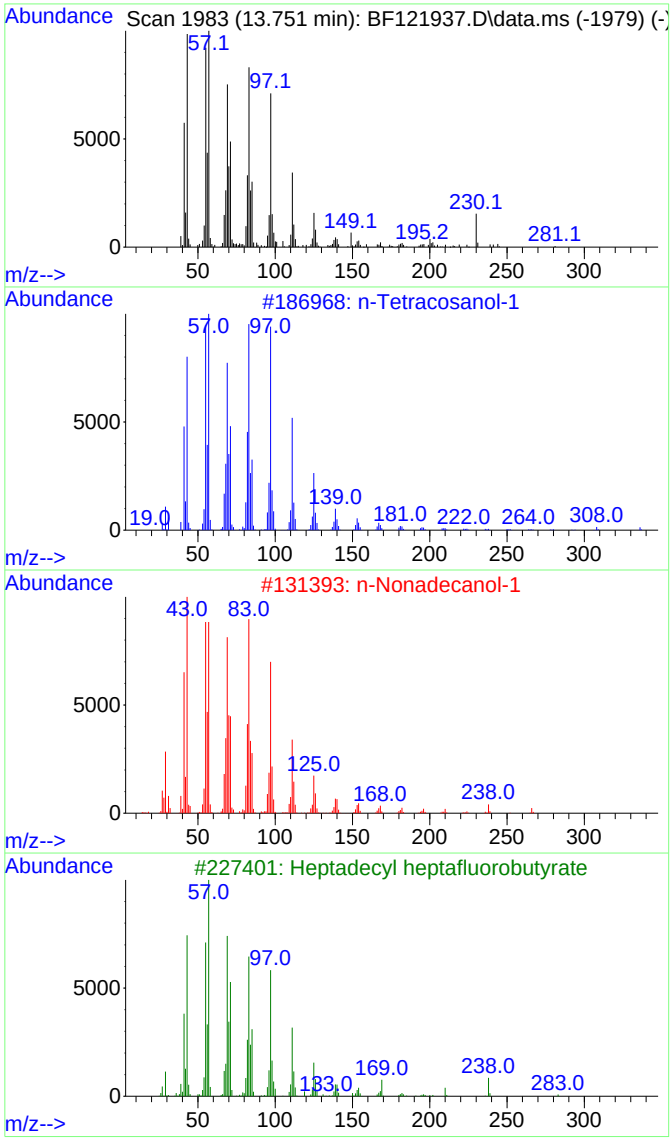
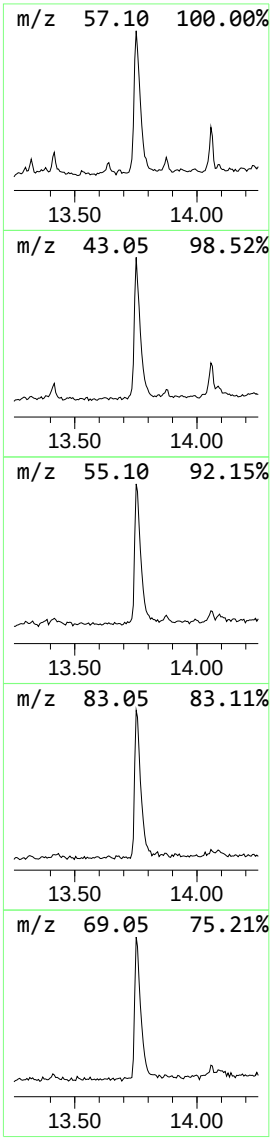
Peak Number 2 n-Tetracosanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	12.08 ng	620062	Chrysene-d12	13.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	Cyclopentadecane	210	C15H30	000295-48-7	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121937.D
Acq On : 13 Oct 2020 14:35
Operator : JU/CG
Sample : L4369-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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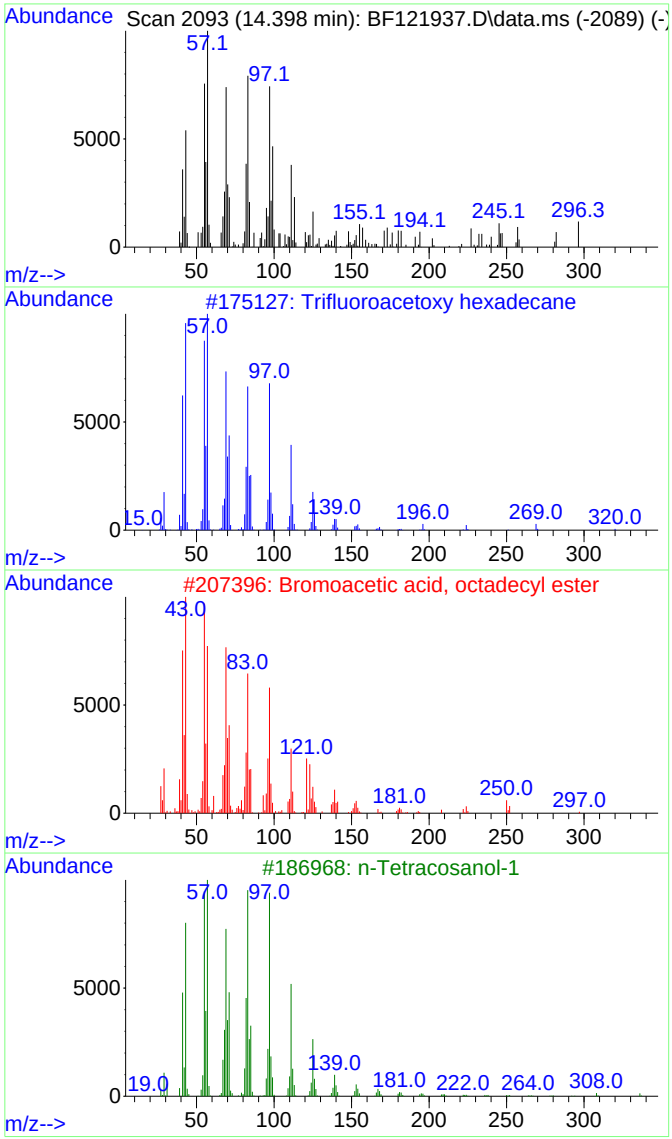
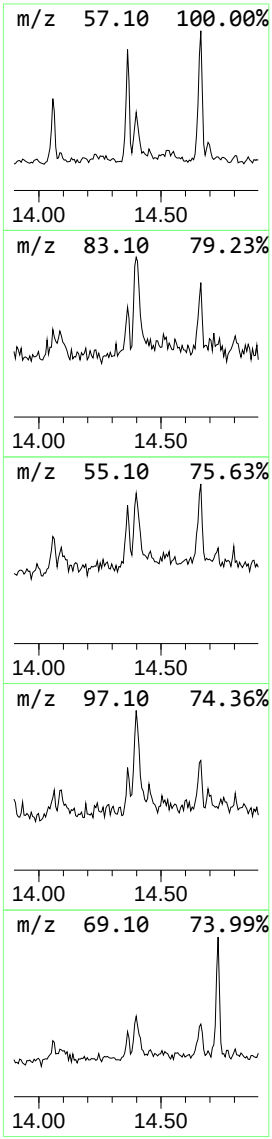
Peak Number 3 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.398	2.90 ng	148772	Chrysene-d12	13.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	64
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	64
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	62
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121937.D
Acq On : 13 Oct 2020 14:35
Operator : JU/CG
Sample : L4369-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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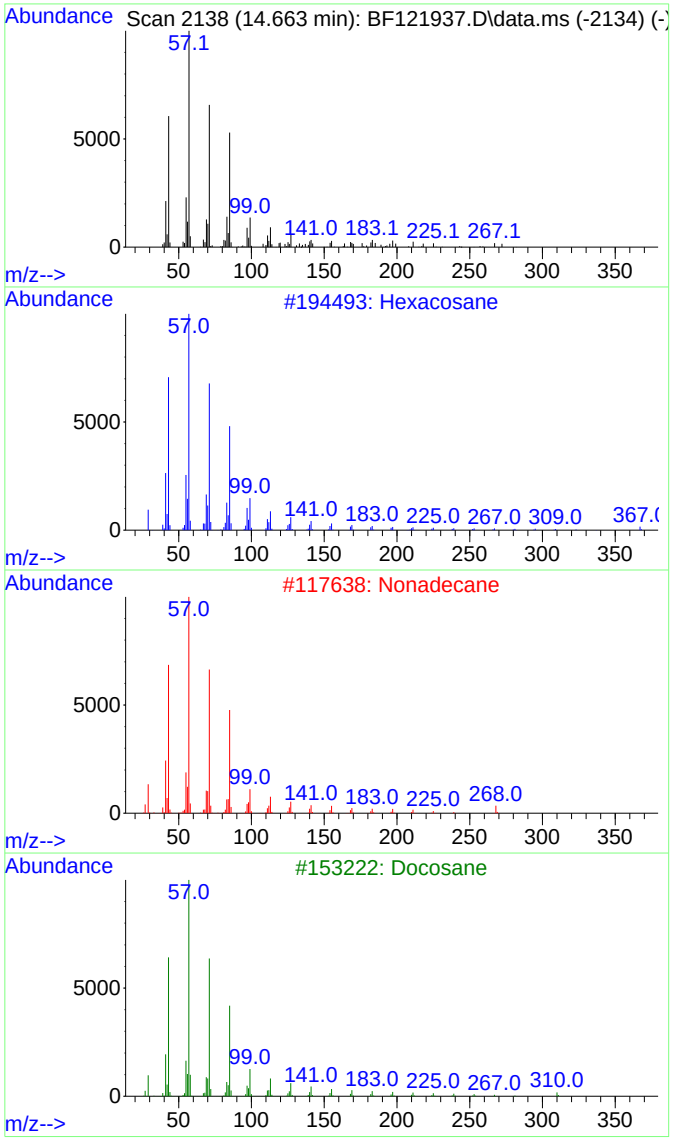
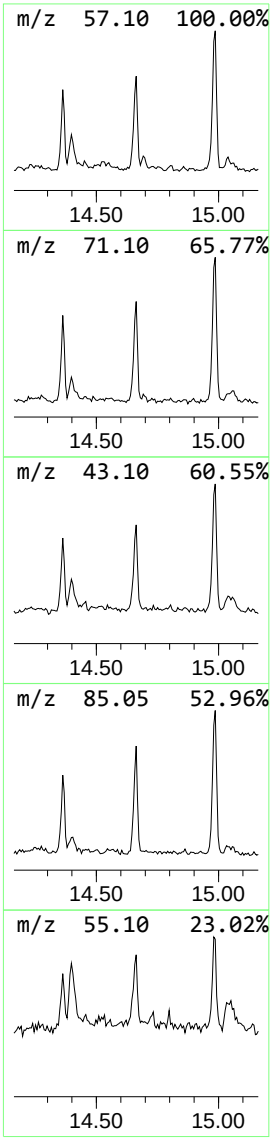
Peak Number 4 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.663	2.34 ng	112854	Perylene-d12	15.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Nonadecane	268	C19H40	000629-92-5	87
3	Docosane	310	C22H46	000629-97-0	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Hexadecane, 5-butyl-	282	C20H42	006912-07-8	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121937.D
Acq On : 13 Oct 2020 14:35
Operator : JU/CG
Sample : L4369-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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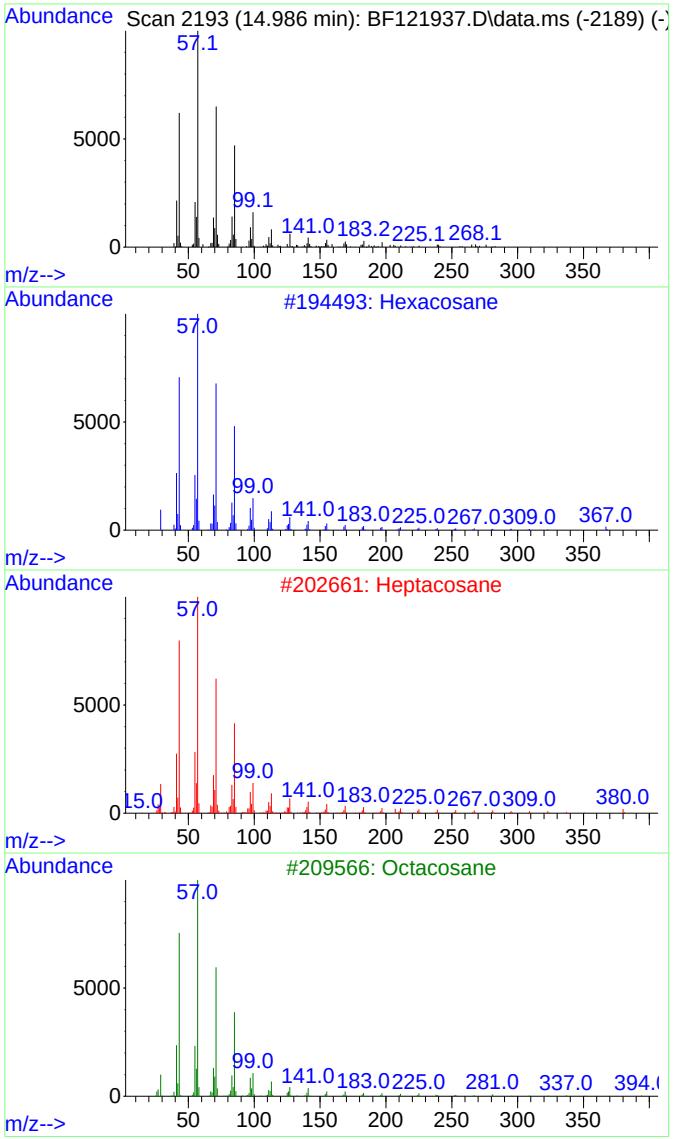
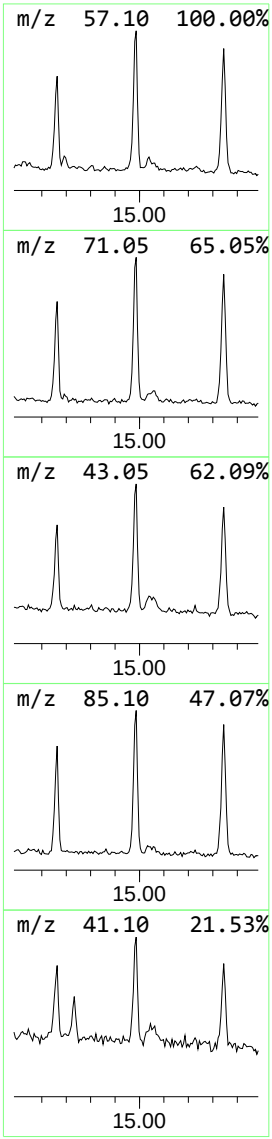
Peak Number 5 Heptacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	4.03 ng	194776	Perylene-d12	15.333

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





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121937.D
Acq On : 13 Oct 2020 14:35
Operator : JU/CG
Sample : L4369-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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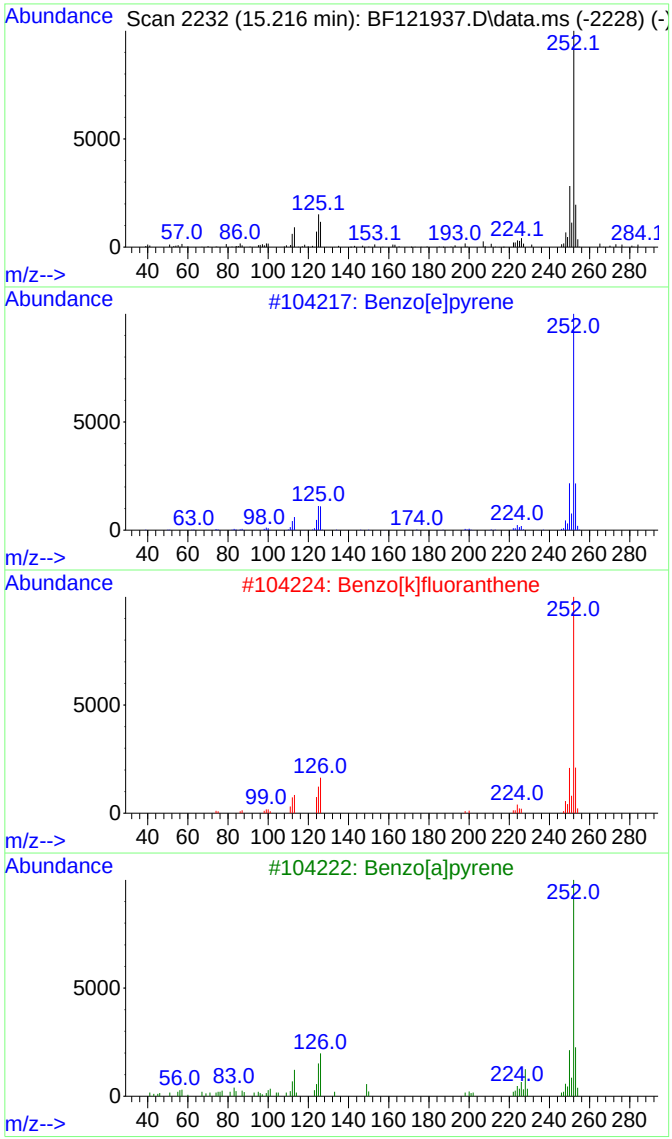
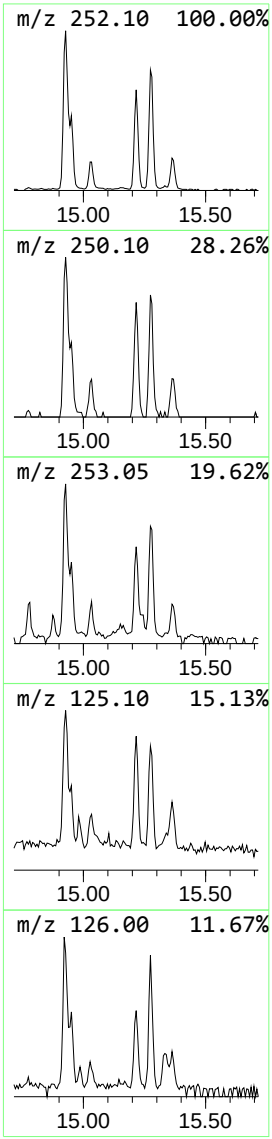
Peak Number 6 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.216	2.26 ng	109407	Perylene-d12	15.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[a]pyrene	252	C20H12	000050-32-8	95
4	Perylene	252	C20H12	000198-55-0	94
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121937.D
Acq On : 13 Oct 2020 14:35
Operator : JU/CG
Sample : L4369-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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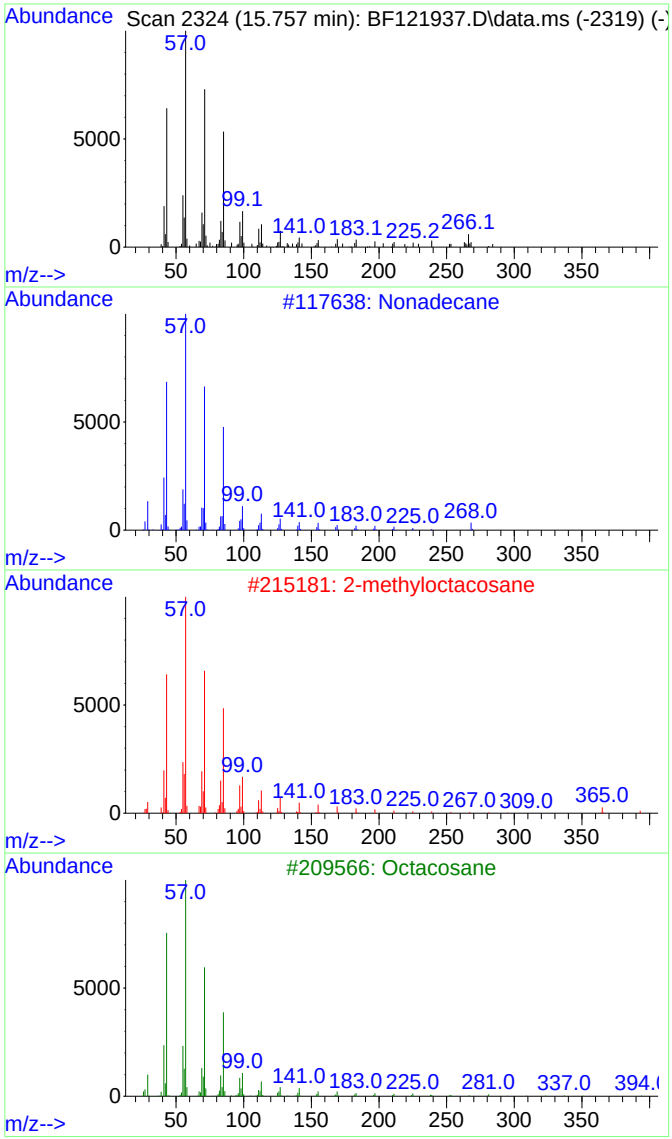
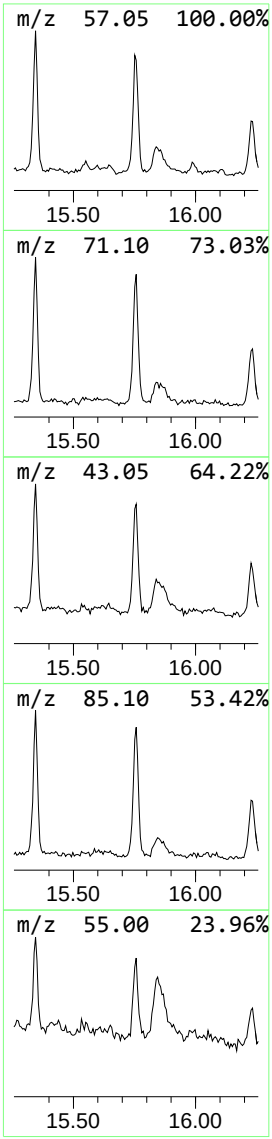
Peak Number 7 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.757	3.77 ng	181927	Perylene-d12	15.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Hexacosane	366	C26H54	000630-01-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121937.D
Acq On : 13 Oct 2020 14:35
Operator : JU/CG
Sample : L4369-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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
n-Hexadecanoic ...	11.792	3.7	ng	205279	4	11.263	1104950	20.0
n-Tetracosanol-1	13.751	12.1	ng	620062	5	13.898	1026320	20.0
Trifluoroacetox...	14.398	2.9	ng	148772	5	13.898	1026320	20.0
Hexacosane	14.663	2.3	ng	112854	6	15.333	966313	20.0
Heptacosane	14.986	4.0	ng	194776	6	15.333	966313	20.0
Benzo[e]pyrene	15.216	2.3	ng	109407	6	15.333	966313	20.0
Nonadecane	15.757	3.8	ng	181927	6	15.333	966313	20.0