LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081122\
Data File : BF129729.D
Acq On : 11 Aug 2022 22:46
Operator : CG\JU
Sample : N3894-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-32

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129729.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	470	473	483	rBV	43686	57082	1.48%	0.200%
2	5.475	538	542	560	rBV	3502957	3314601	86.03%	11.595%
3	6.487	710	714	717	rBV	3586130	3238124	84.04%	11.327%
4	6.834	769	773	776	rBV	993027	900207	23.36%	3.149%
5	7.398	864	869	872	rBV	2335495	2147954	55.75%	7.514%
6	8.116	987	991	994	rBV	1350049	1160279	30.11%	4.059%
7	9.186	1168	1173	1176	rBV	4291306	3852965	100.00%	13.478%
8	9.869	1285	1289	1292	rBV	1469556	1132862	29.40%	3.963%
9	10.663	1420	1424	1427	rBV	2094386	1679840	43.60%	5.876%
10	10.757	1437	1440	1445	rBV	55846	50071	1.30%	0.175%
11	11.357	1539	1542	1545	rBV	1082983	912310	23.68%	3.191%
12	11.380	1545	1546	1552	rVB	130317	102366	2.66%	0.358%
13	11.880	1623	1631	1638	rBV3	62126	141095	3.66%	0.494%
14	12.574	1746	1749	1753	rVB	311157	253467	6.58%	0.887%
15	12.786	1782	1785	1786	rBV2	53795	51714	1.34%	0.181%
16	12.804	1786	1788	1794	rVB	318123	274056	7.11%	0.959%
17	12.945	1808	1812	1815	rBV	3260892	2706724	70.25%	9.468%
18	13.021	1821	1825	1829	rBV4	29097	49659	1.29%	0.174%
19	13.221	1856	1859	1864	rVB3	122595	139590	3.62%	0.488%
20	13.368	1880	1884	1889	rBV3	29918	60513	1.57%	0.212%
21	13.645	1929	1931	1936	rVB	48200	41923	1.09%	0.147%
22	13.863	1964	1968	1984	rVB5	138123	402924	10.46%	1.409%
23	14.010	1988	1993	1995	rVV2	899519	989635	25.69%	3.462%
24	14.033	1995	1997	2000	rVB	198919	152389	3.96%	0.533%
25	14.098	2004	2008	2013	rBV2	109800	125620	3.26%	0.439%
26	14.274	2035	2038	2040	rBV3	50311	46028	1.19%	0.161%
27	14.451	2065	2068	2073	rVB	129470	116428	3.02%	0.407%
28	14.515	2076	2079	2082	rBV3	67518	92987	2.41%	0.325%
29	14.751	2117	2119	2122	rVB2	66977	65774	1.71%	0.230%
30	14.833	2130	2133	2136	rVB	52436	52534	1.36%	0.184%
31	14.904	2141	2145	2150	rVB2	300907	319459	8.29%	1.117%
32	15.051	2166	2170	2173	rBV	181913	263005	6.83%	0.920%
33	15.086	2173	2176	2181	rVB2	394166	472508	12.26%	1.653%
34	15.168	2185	2190	2201	rBV6	163527	557022	14.46%	1.948%
35	15.357	2218	2222	2226	rVB	110173	138426	3.59%	0.484%
36	15.415	2229	2232	2236	rVB	145340	162596	4.22%	0.569%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081122\
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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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.480	2237	2243	2247	rBV	558371	731019	18.97%	2.557%
38	15.668	2271	2275	2280	rBV	148175	186295	4.84%	0.652%
39	15.892	2309	2313	2322	rVB	316845	478726	12.42%	1.675%
40	16.686	2444	2448	2457	rVB2	129148	224158	5.82%	0.784%
41	16.968	2490	2496	2505	rBV3	110395	287461	7.46%	1.006%
42	17.074	2508	2514	2520	rVB6	157331	340754	8.84%	1.192%
43	17.580	2596	2600	2607	rVB9	55790	114385	2.97%	0.400%

Sum of corrected areas: 28587535

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081122\
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Instrument :
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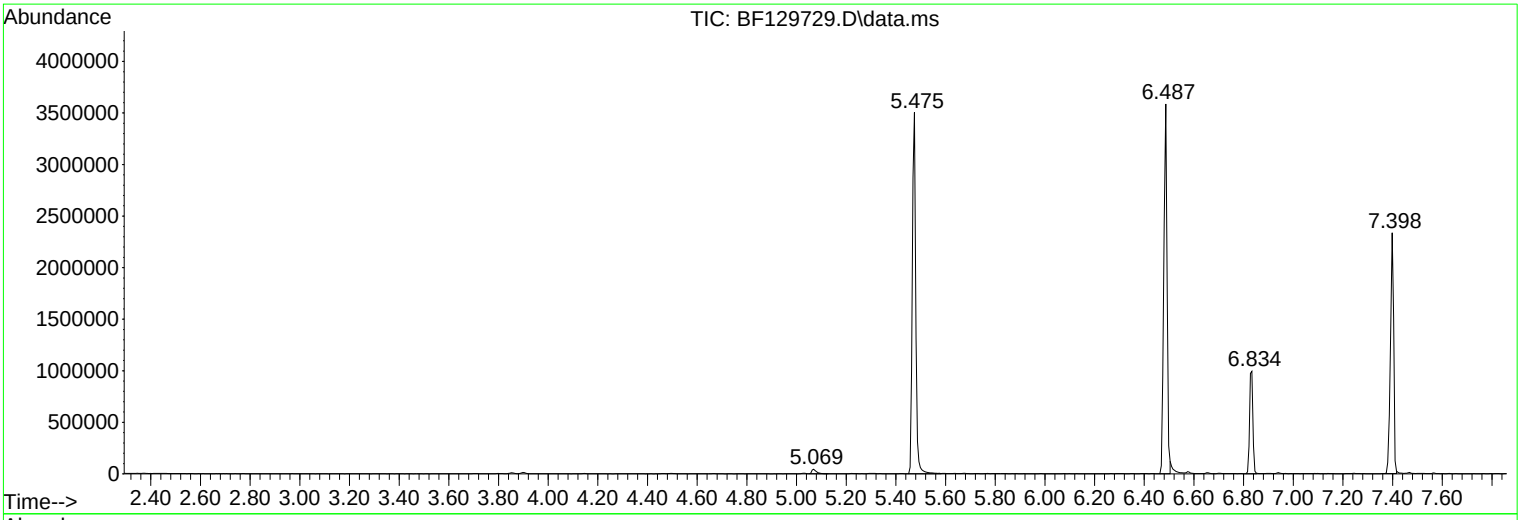
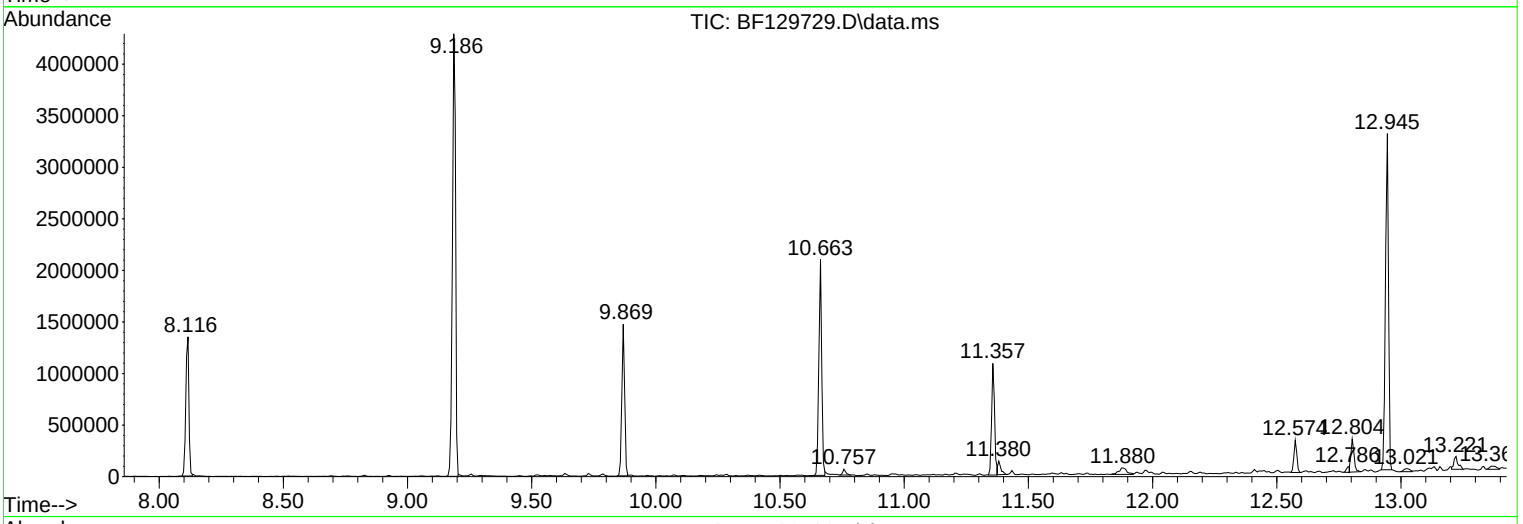
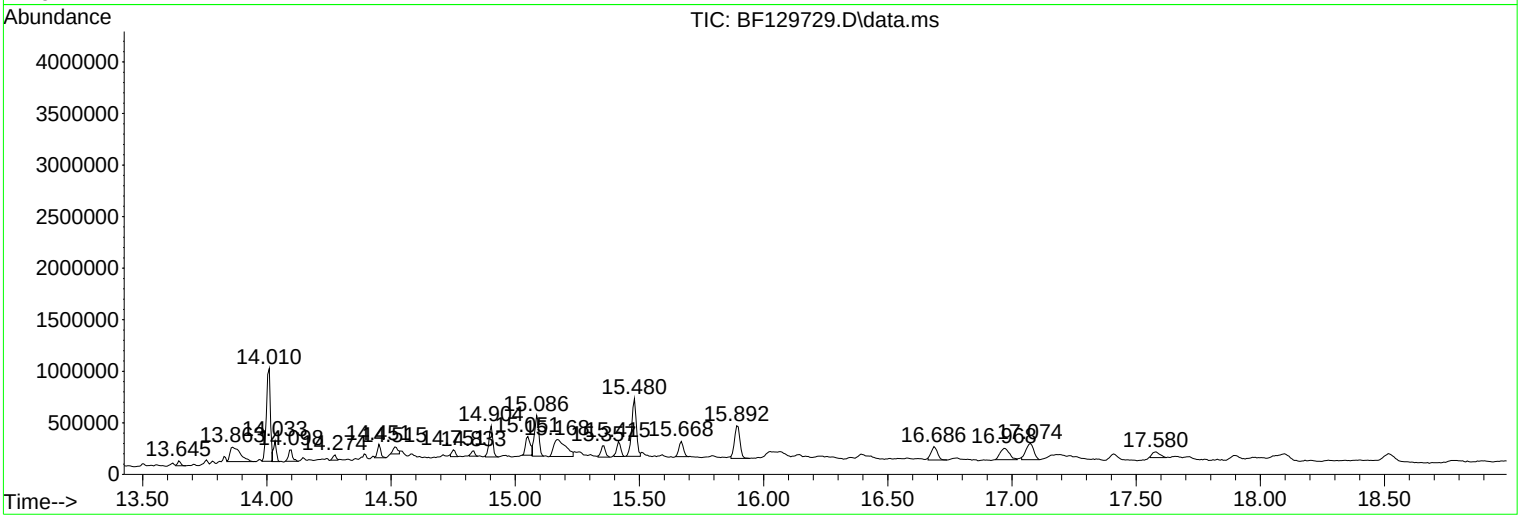
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Data File : BF129729.D
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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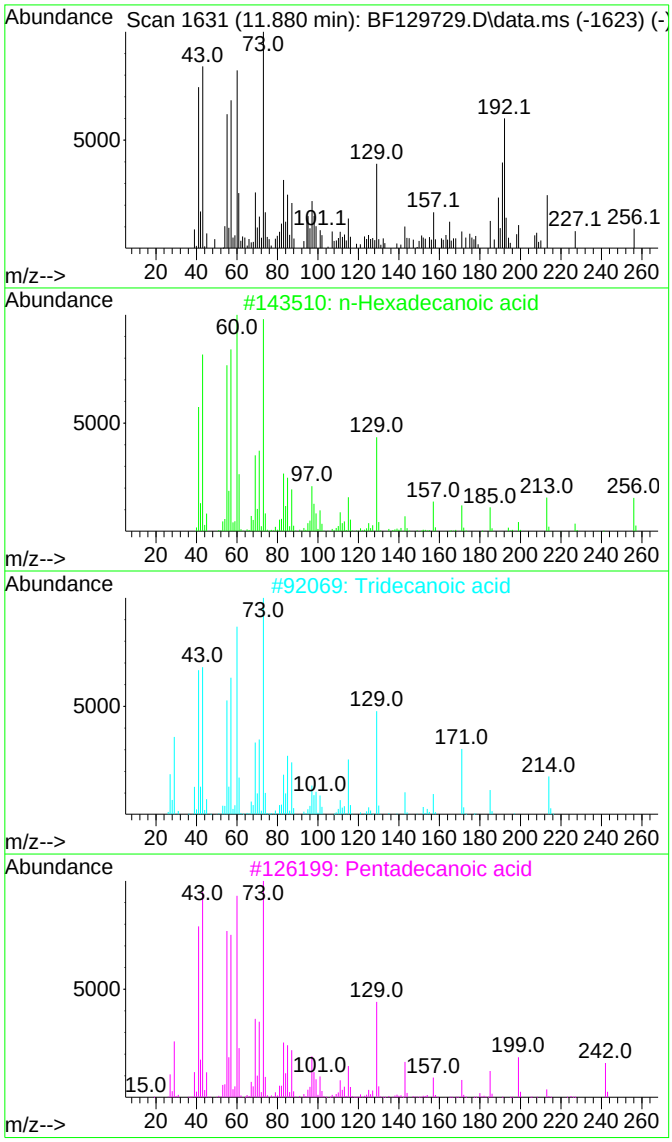
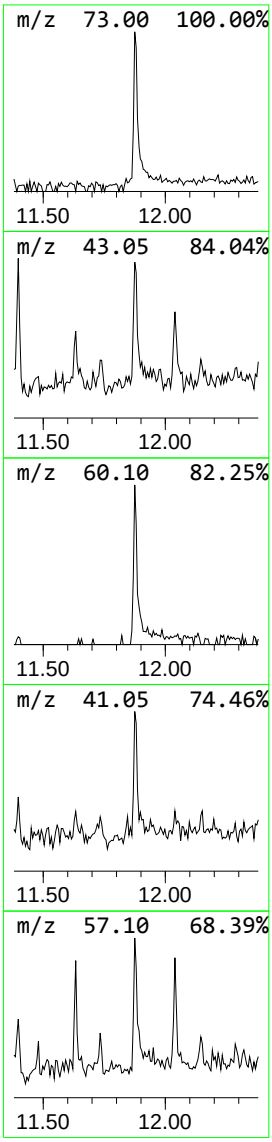
Peak Number 1 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	3.09 ng	141095	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	49
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	40
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	40





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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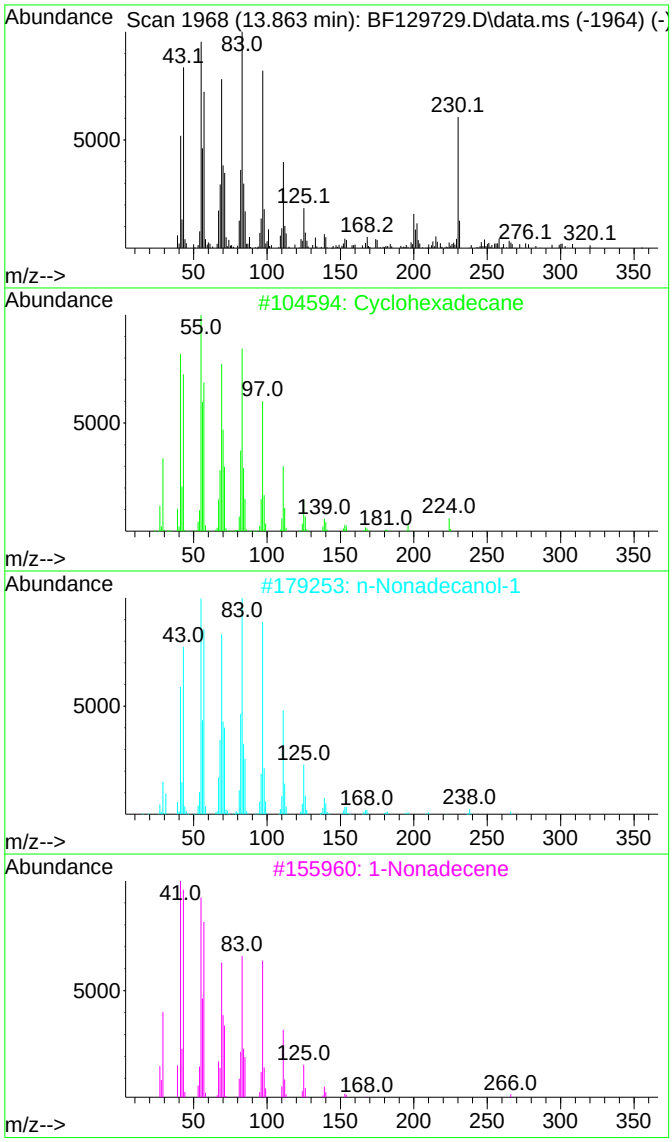
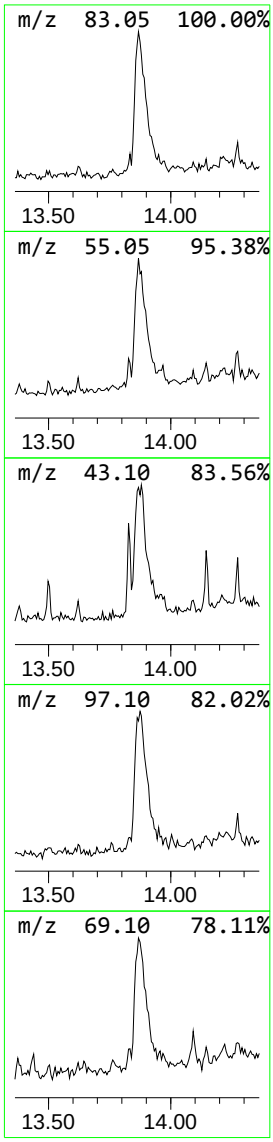
Peak Number 3 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	8.14 ng	402924	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
5	1-Octadecanol	270	C18H38O	000112-92-5	87





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Data File : BF129729.D
Acq On : 11 Aug 2022 22:46
Operator : CG\JU
Sample : N3894-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-32

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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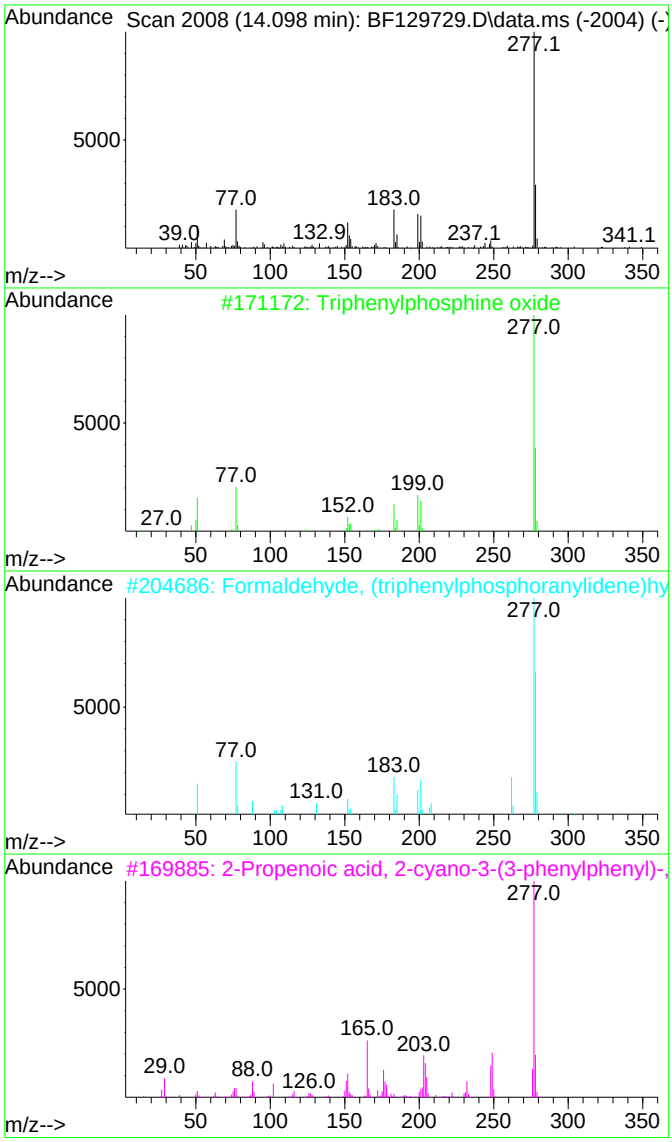
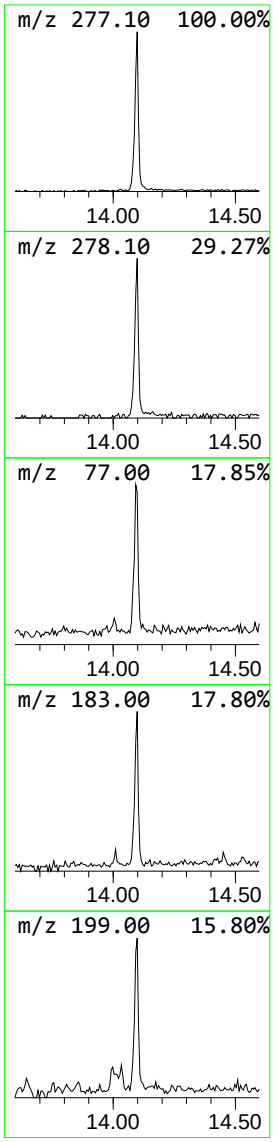
Peak Number 4 Triphenylphosphine oxide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	2.54 ng	125620	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	68
3	2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	59
4	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	50
5	Dimethoxymethyl-hydroxy-tripheny...	354	C21H23O3P	1000132-00-1	42





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Data File : BF129729.D
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Sample : N3894-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-32

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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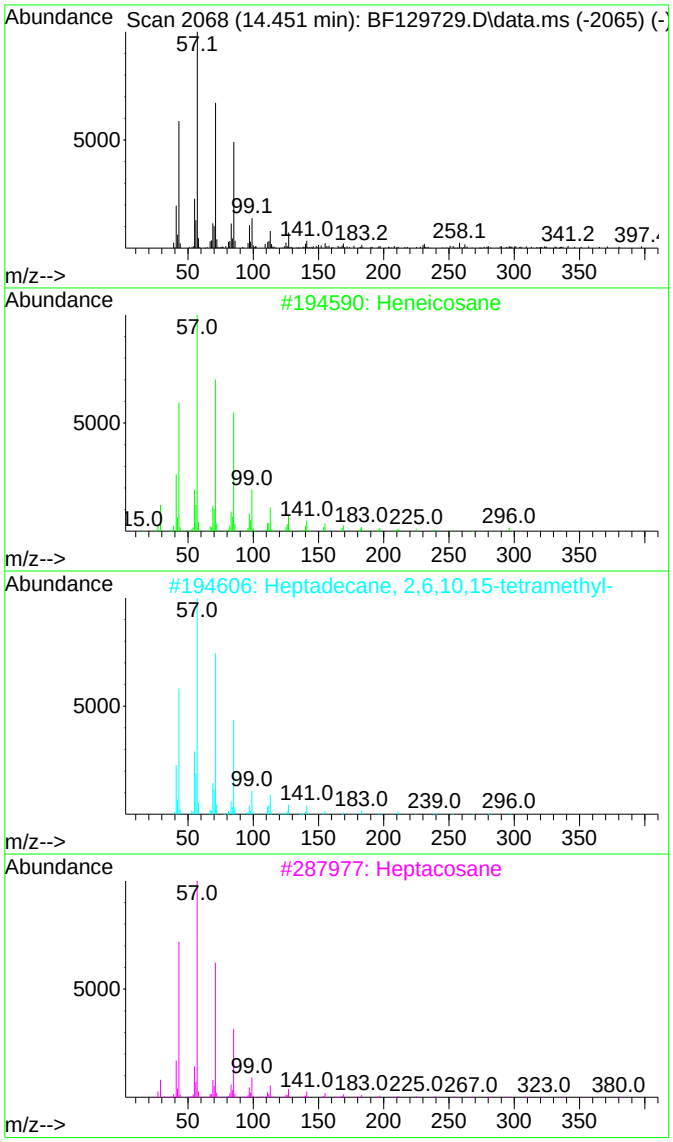
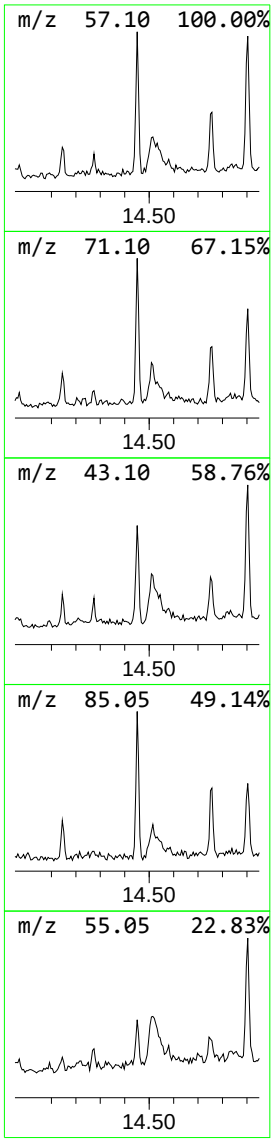
Peak Number 5 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	2.35 ng	116428	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3	Heptacosane	380	C27H56	000593-49-7	93
4	Octacosane	394	C28H58	000630-02-4	87
5	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	86





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Operator : CG\JU
Sample : N3894-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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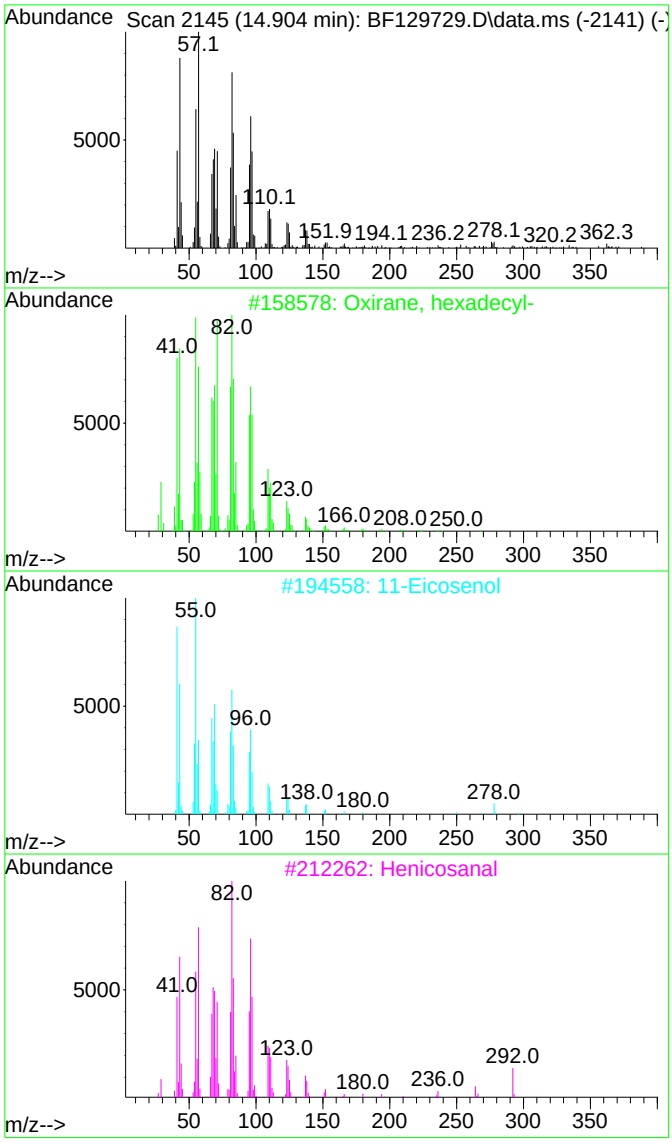
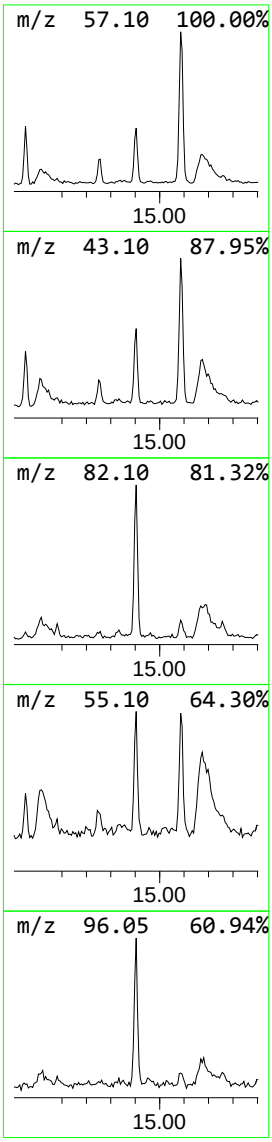
Peak Number 6 Oxirane, hexadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	8.74 ng	319459	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2	11-Eicosenol	296	C20H40O	1010424-20-3	93
3	Henicosanal	310	C21H42O	051227-32-8	93
4	Hexacosanal	380	C26H52O	026627-85-0	93
5	Eicosanal-	296	C20H40O	002400-66-0	93





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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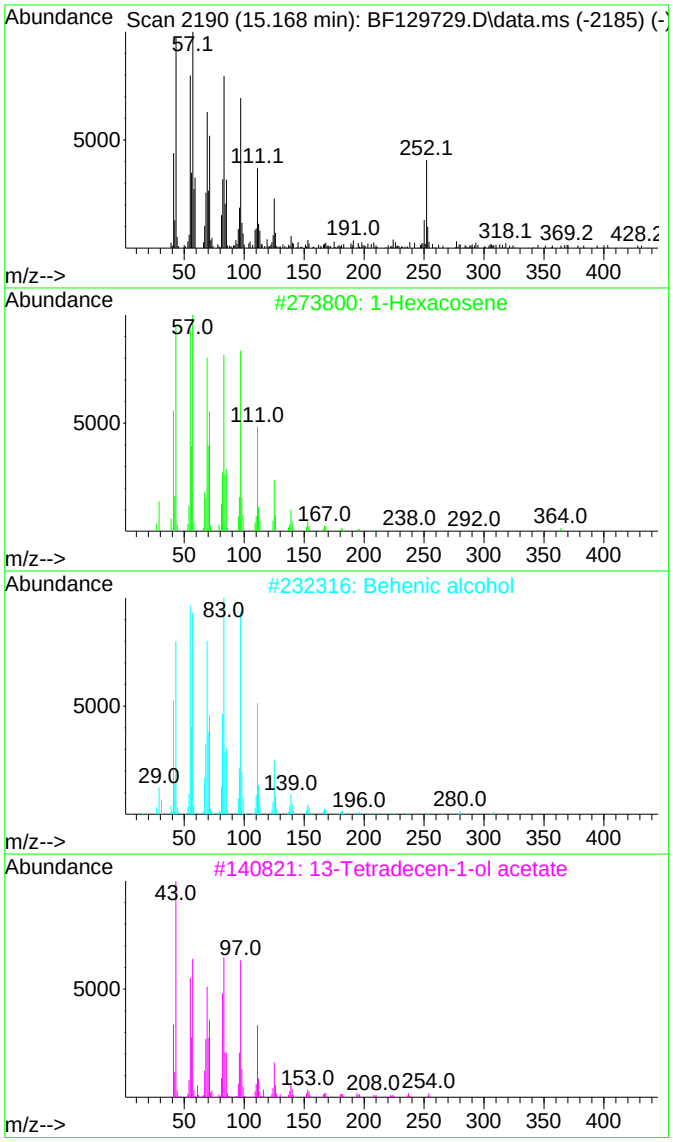
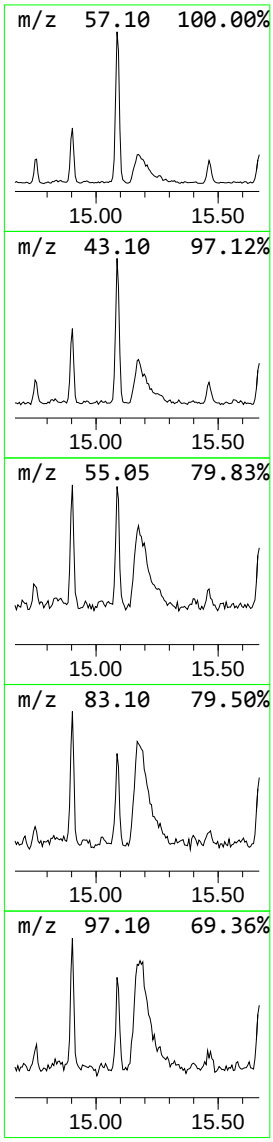
Peak Number 7 1-Hexacosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.168	15.24 ng	557022	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	95
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	89
5	Heptadecafluorononanoic acid, oc...	716	C27H37F17O2	1000356-03-4	87





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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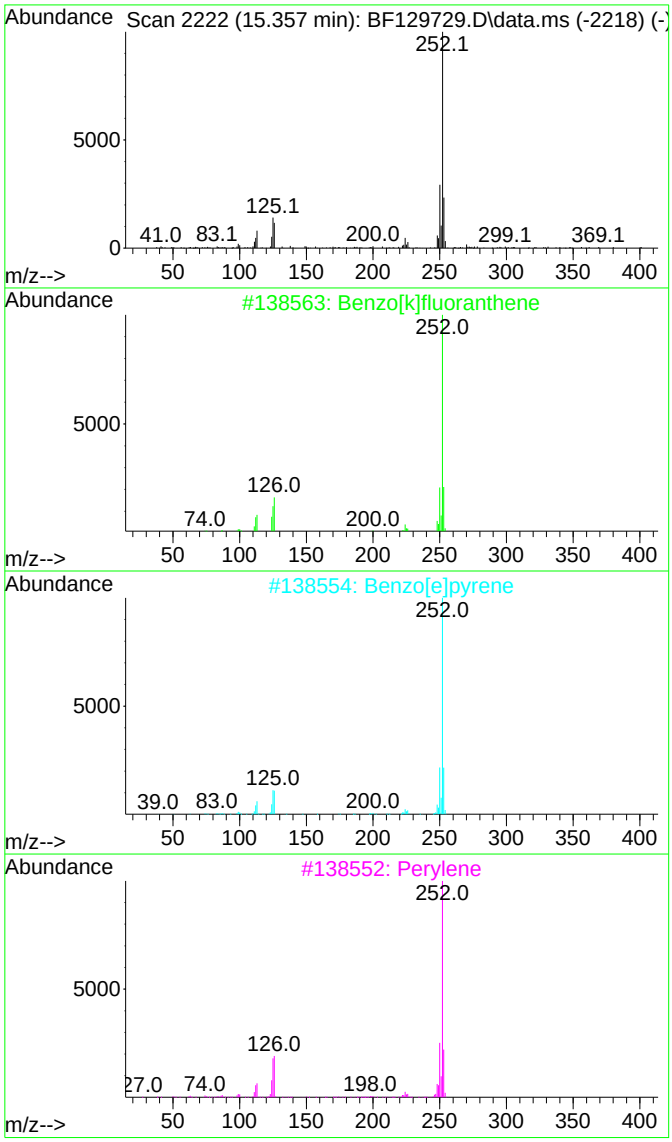
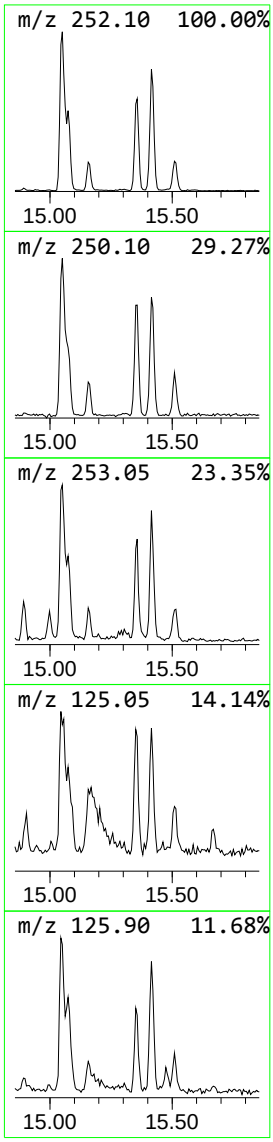
Peak Number 8 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.357	3.79 ng	138426	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
2	Benzo[e]pyrene	252	C20H12	000192-97-2	97
3	Perylene	252	C20H12	000198-55-0	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





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Operator : CG\JU
Sample : N3894-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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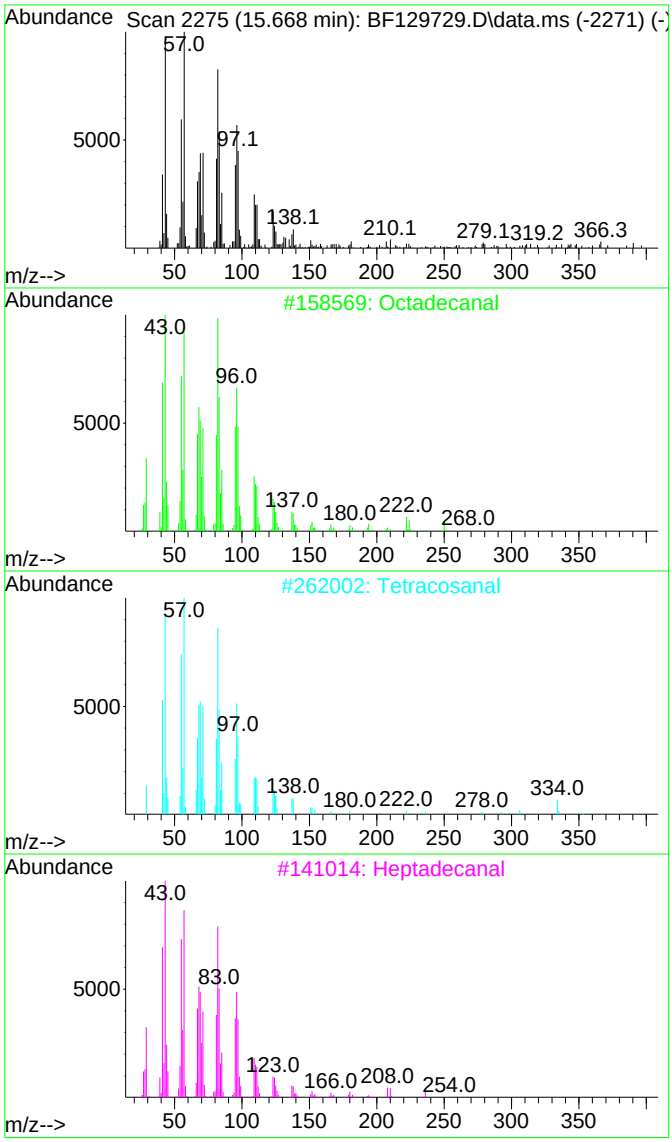
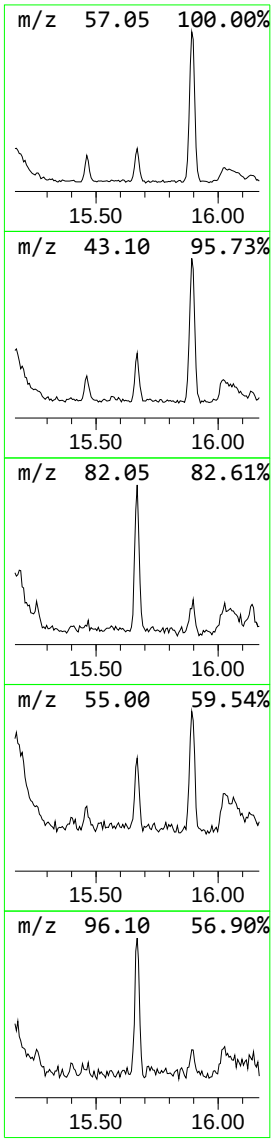
Peak Number 9 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.668	5.10 ng	186295	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	94
2	Tetracosanal	352	C24H48O	057866-08-7	94
3	Heptadecanal	254	C17H34O	1000376-70-0	94
4	1,19-Eicosadiene	278	C20H38	014811-95-1	93
5	Docosanal	324	C22H44O	057402-36-5	91





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Acq On : 11 Aug 2022 22:46
Operator : CG\JU
Sample : N3894-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-32

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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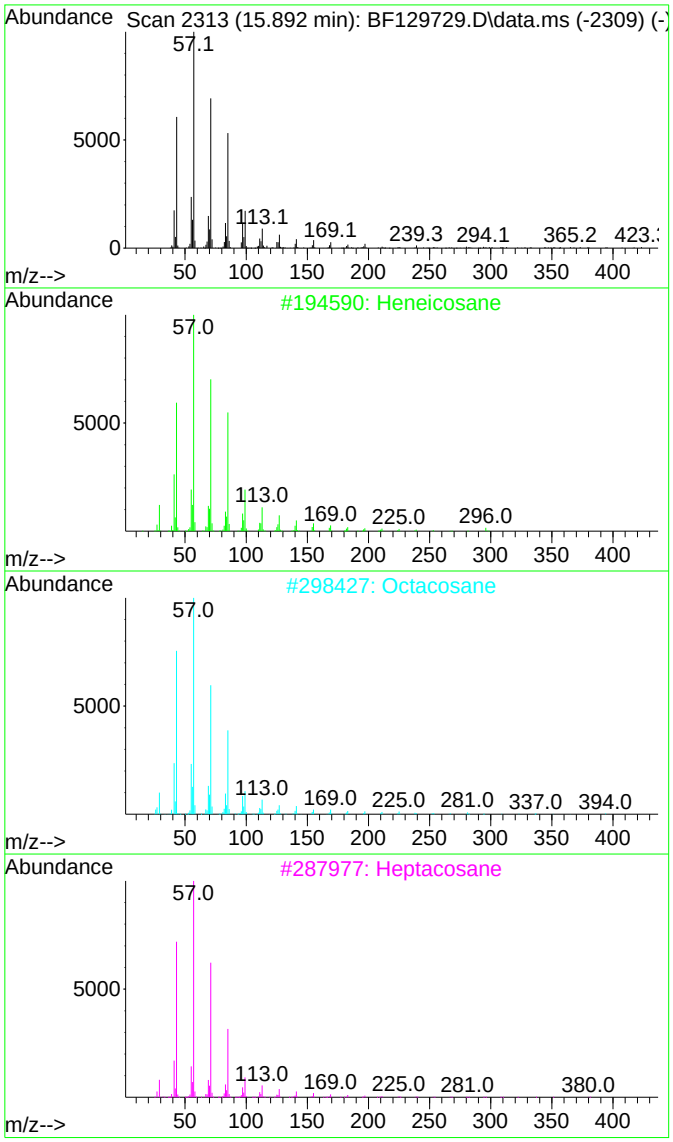
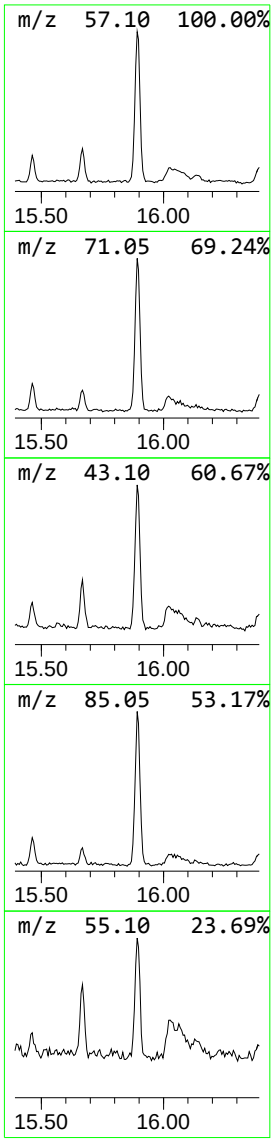
Peak Number 10 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	13.10 ng	478726	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Octacosane	394	C28H58	000630-02-4	94
3	Heptacosane	380	C27H56	000593-49-7	94
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
5	Pentacosane	352	C25H52	000629-99-2	91





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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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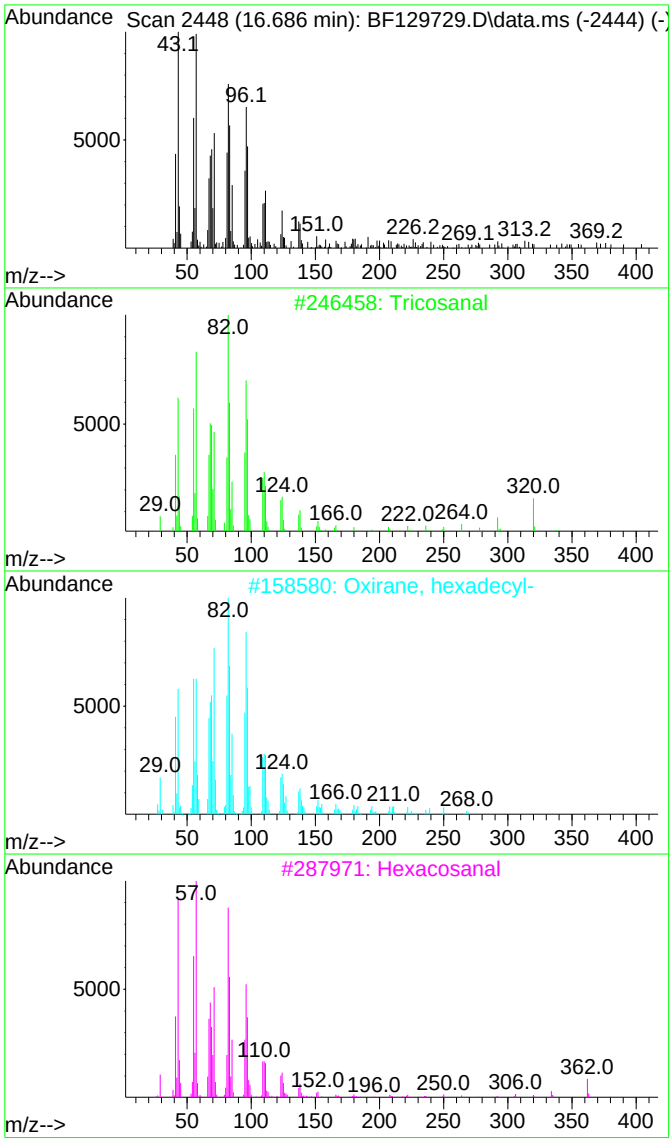
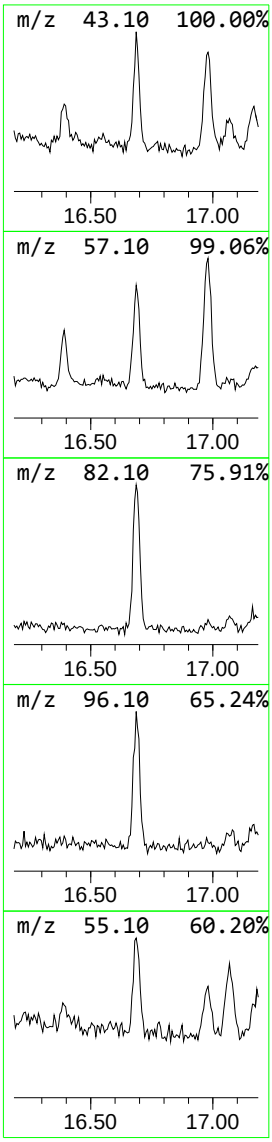
Peak Number 11 Tricosanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.686	6.13 ng	224158	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosanal	338	C23H46O	072934-02-2	94
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Hexacosanal	380	C26H52O	026627-85-0	91
4	Octadecanal	268	C18H36O	000638-66-4	91
5	1,19-Eicosadiene	278	C20H38	014811-95-1	90





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Operator : CG\JU
Sample : N3894-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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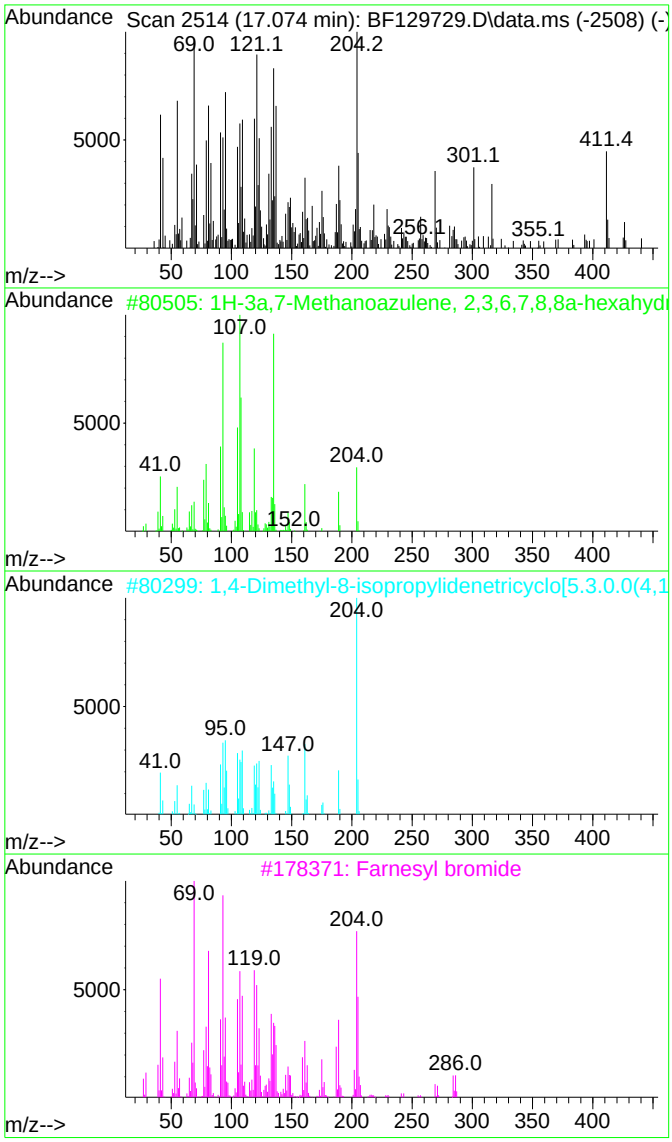
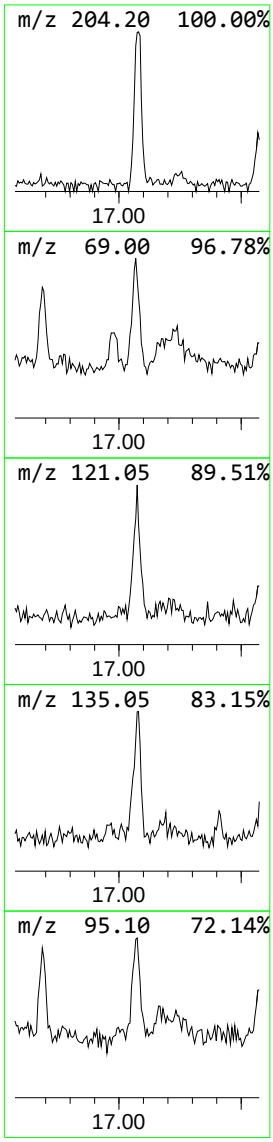
Peak Number 12 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.074	9.32 ng	340754	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	50
2	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	47
3	Farnesyl bromide	284	C15H25Br	006874-67-5	44
4	1-Naphthalenecarboxylic acid, de...	316	C21H32O2	001235-39-8	41
5	Neointermedeol	222	C15H26O	005945-72-2	38





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Operator : CG\JU
Sample : N3894-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-32

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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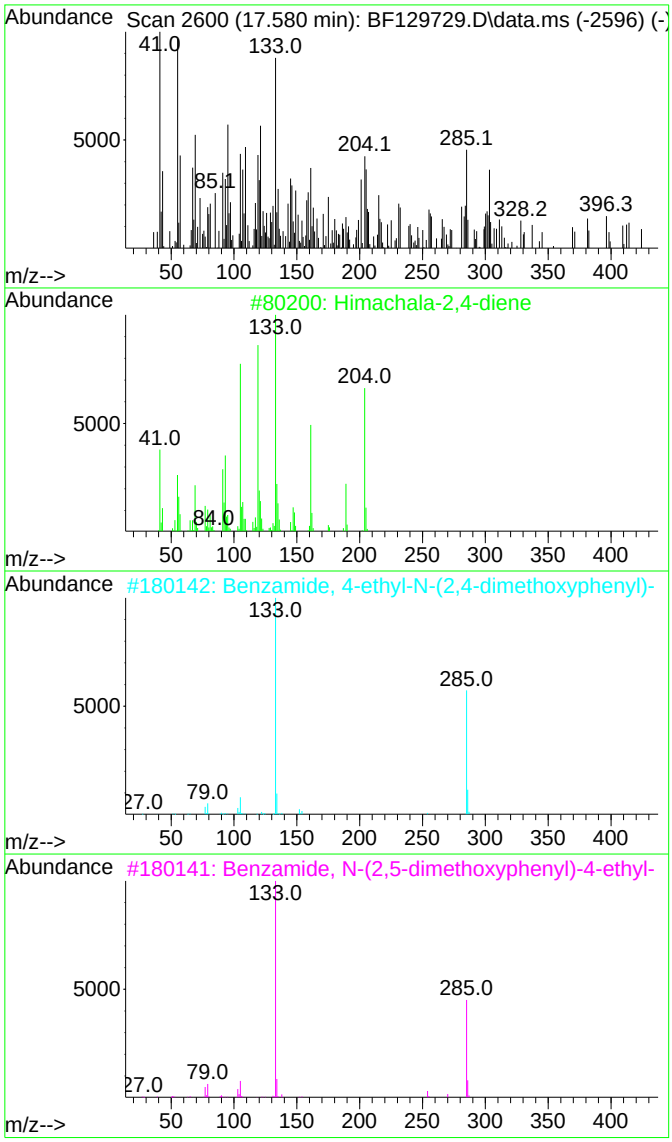
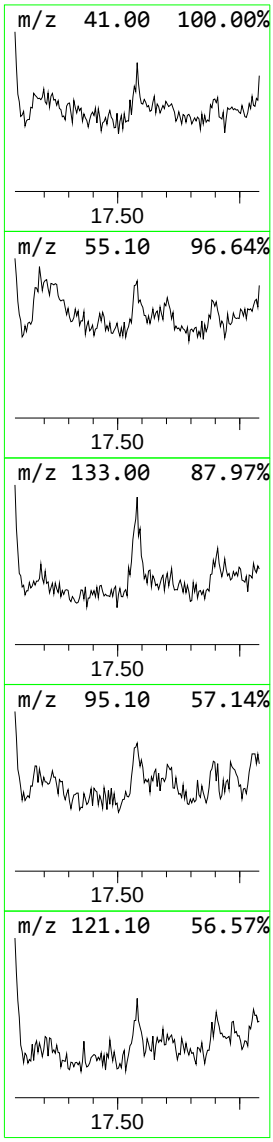
Peak Number 13 unknown17.580 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.580	3.13 ng	114385	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Himachala-2,4-diene	204	C15H24	060909-27-5	38
2	Benzamide, 4-ethyl-N-(2,4-dimeth...	285	C17H19NO3	1000340-35-3	30
3	Benzamide, N-(2,5-dimethoxypheny...	285	C17H19NO3	1000307-01-8	27
4	1,2-Bis[methyl(trimethylene)sily...	244	C11H24O2Si2	1000217-00-2	27
5	2-tert-Butylaniline, N-toluenesu...	303	C17H21NO2S	1000467-61-2	25





Tentatively Identified Compound (LSC) summary

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Data File : BF129729.D
Acq On : 11 Aug 2022 22:46
Operator : CG\JU
Sample : N3894-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-32

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	11.880	3.1	ng	141095	4	11.357	912310	20.0
Cyclohexadecane	13.863	8.1	ng	402924	5	14.010	989635	20.0
Triphenylphosph...	14.098	2.5	ng	125620	5	14.010	989635	20.0
Heneicosane	14.451	2.4	ng	116428	5	14.010	989635	20.0
Oxirane, hexade...	14.904	8.7	ng	319459	6	15.480	731019	20.0
1-Hexacosene	15.168	15.2	ng	557022	6	15.480	731019	20.0
Benzo[e]pyrene	15.357	3.8	ng	138426	6	15.480	731019	20.0
Octadecanal	15.668	5.1	ng	186295	6	15.480	731019	20.0
Octacosane	15.892	13.1	ng	478726	6	15.480	731019	20.0
Tricosanal	16.686	6.1	ng	224158	6	15.480	731019	20.0
1H-3a,7-Methano...	17.074	9.3	ng	340754	6	15.480	731019	20.0
unknown17.580	17.580	3.1	ng	114385	6	15.480	731019	20.0