LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF130005.D
Acq On : 25 Aug 2022 18:19
Operator : CG\JU
Sample : N4352-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11985

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130005.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.969	453	456	478	rBV	391325	504172	21.14%	2.469%
2	5.393	525	528	554	rBV	2027197	2275439	95.43%	11.141%
3	5.775	589	593	600	rVB	34457	38125	1.60%	0.187%
4	6.416	699	702	717	rBV	2423711	2191022	91.89%	10.728%
5	6.757	756	760	767	rBV	716376	635986	26.67%	3.114%
6	7.328	853	857	864	rBV	1500045	1420164	59.56%	6.954%
7	8.034	974	977	983	rBV	878097	796010	33.38%	3.898%
8	9.110	1156	1160	1163	rBV	3055730	2384430	100.00%	11.675%
9	9.651	1249	1252	1256	rBV	27873	29171	1.22%	0.143%
10	9.786	1272	1275	1279	rBV	992132	784721	32.91%	3.842%
11	10.581	1407	1410	1424	rBV	1354948	1215353	50.97%	5.951%
12	10.704	1429	1431	1439	rVB	33525	32029	1.34%	0.157%
13	11.275	1525	1528	1531	rBV	726188	658394	27.61%	3.224%
14	11.304	1531	1533	1538	rVB	151015	132148	5.54%	0.647%
15	11.357	1538	1542	1546	rBV	35083	32734	1.37%	0.160%
16	11.657	1590	1593	1596	rBV	41294	31083	1.30%	0.152%
17	11.780	1610	1614	1615	rBV	36474	31546	1.32%	0.154%
18	11.804	1615	1618	1625	rVB3	196896	230395	9.66%	1.128%
19	11.892	1630	1633	1635	rBV	49865	47229	1.98%	0.231%
20	12.327	1704	1707	1710	rBV	36088	37737	1.58%	0.185%
21	12.433	1720	1725	1732	rVB2	24704	37668	1.58%	0.184%
22	12.492	1732	1735	1739	rBV	336098	292563	12.27%	1.433%
23	12.586	1748	1751	1758	rBV2	75021	101286	4.25%	0.496%
24	12.722	1768	1774	1779	rBV	277137	301290	12.64%	1.475%
25	12.857	1793	1797	1801	rBV	1919347	1771960	74.31%	8.676%
26	12.945	1807	1812	1817	rBV4	28571	48030	2.01%	0.235%
27	13.057	1823	1831	1837	rBV	47395	85732	3.60%	0.420%
28	13.122	1839	1842	1845	rBV	32194	29641	1.24%	0.145%
29	13.157	1845	1848	1852	rVB2	32892	39763	1.67%	0.195%
30	13.251	1861	1864	1867	rBV2	33516	34042	1.43%	0.167%
31	13.286	1867	1870	1875	rVB3	23203	37551	1.57%	0.184%
32	13.680	1931	1937	1939	rBV2	47650	68424	2.87%	0.335%
33	13.745	1946	1948	1952	rVB2	44051	36252	1.52%	0.178%
34	13.798	1952	1957	1968	rBV6	83630	307360	12.89%	1.505%
35	13.880	1969	1971	1974	rVV	92325	93666	3.93%	0.459%
36	13.922	1974	1978	1982	rVV2	783183	945315	39.65%	4.629%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
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Operator : CG\JU
Sample : N4352-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
11985

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.951	1982	1983	1990	rVV	180410	133338	5.59%	0.653%
38	14.010	1990	1993	2000	rVB2	175139	197771	8.29%	0.968%
39	14.316	2043	2045	2048	rVB	43026	34626	1.45%	0.170%
40	14.369	2048	2054	2056	rBV4	48754	72259	3.03%	0.354%
41	14.439	2064	2066	2068	rBV2	33765	35479	1.49%	0.174%
42	14.733	2113	2116	2120	rVB2	58544	57219	2.40%	0.280%
43	14.804	2125	2128	2133	rBV2	109717	115377	4.84%	0.565%
44	14.957	2150	2154	2156	rBV	201871	253890	10.65%	1.243%
45	14.980	2156	2158	2165	rVB	235762	254843	10.69%	1.248%
46	15.068	2170	2173	2175	rBV	41860	53101	2.23%	0.260%
47	15.251	2201	2204	2211	rVB	116750	140201	5.88%	0.686%
48	15.316	2211	2215	2221	rBV	156185	214336	8.99%	1.049%
49	15.368	2221	2224	2229	rBV2	538526	660029	27.68%	3.232%
50	15.539	2250	2253	2258	rVB5	42656	55425	2.32%	0.271%
51	15.751	2285	2289	2295	rVB	131748	183048	7.68%	0.896%
52	16.510	2415	2418	2426	rVB7	40076	73119	3.07%	0.358%
53	16.821	2468	2471	2477	rVB	55742	83655	3.51%	0.410%
54	17.257	2542	2545	2553	rVB2	36724	66964	2.81%	0.328%

Sum of corrected areas: 20423111

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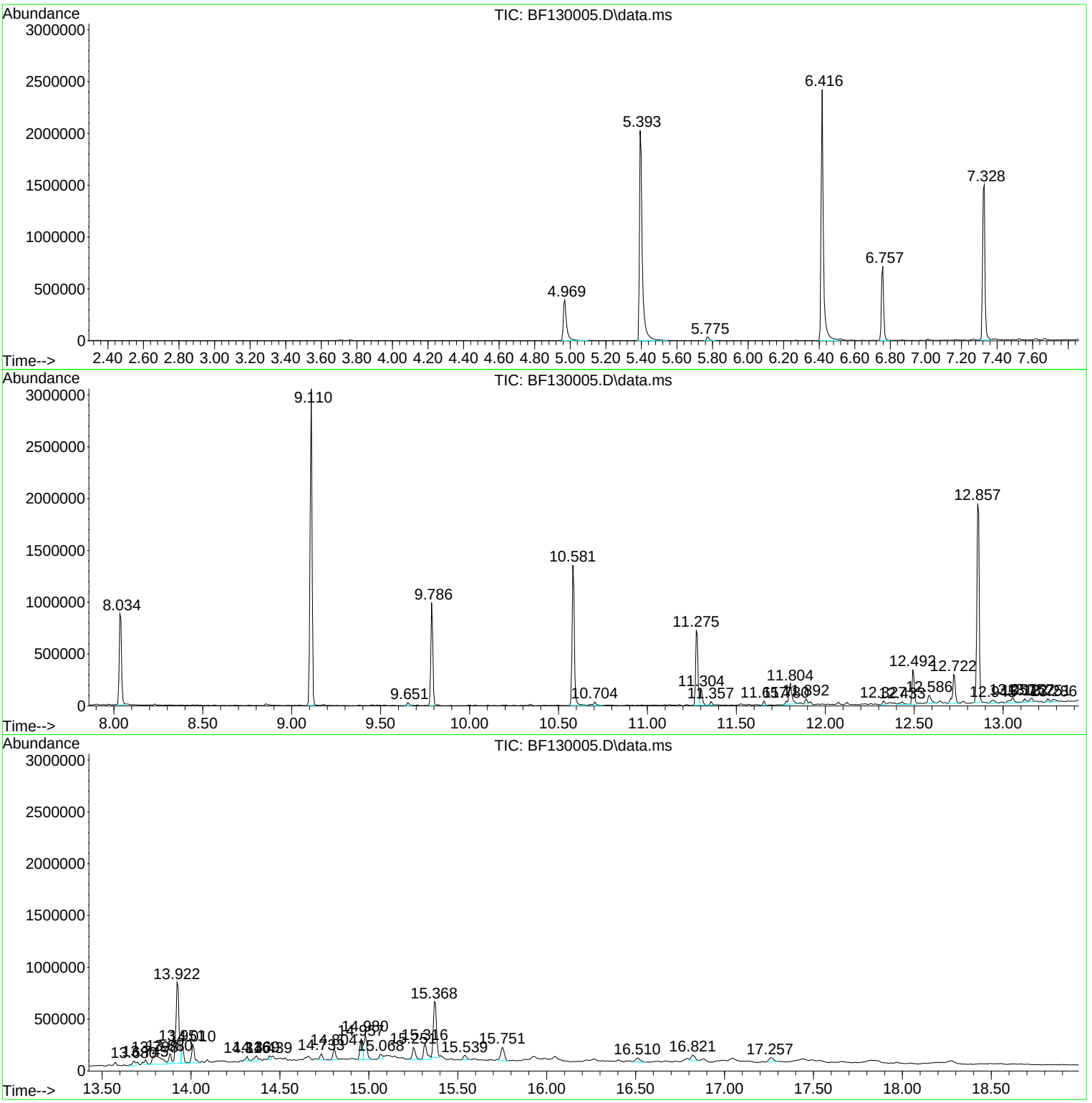
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
11985

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF130005.D
Acq On : 25 Aug 2022 18:19
Operator : CG\JU
Sample : N4352-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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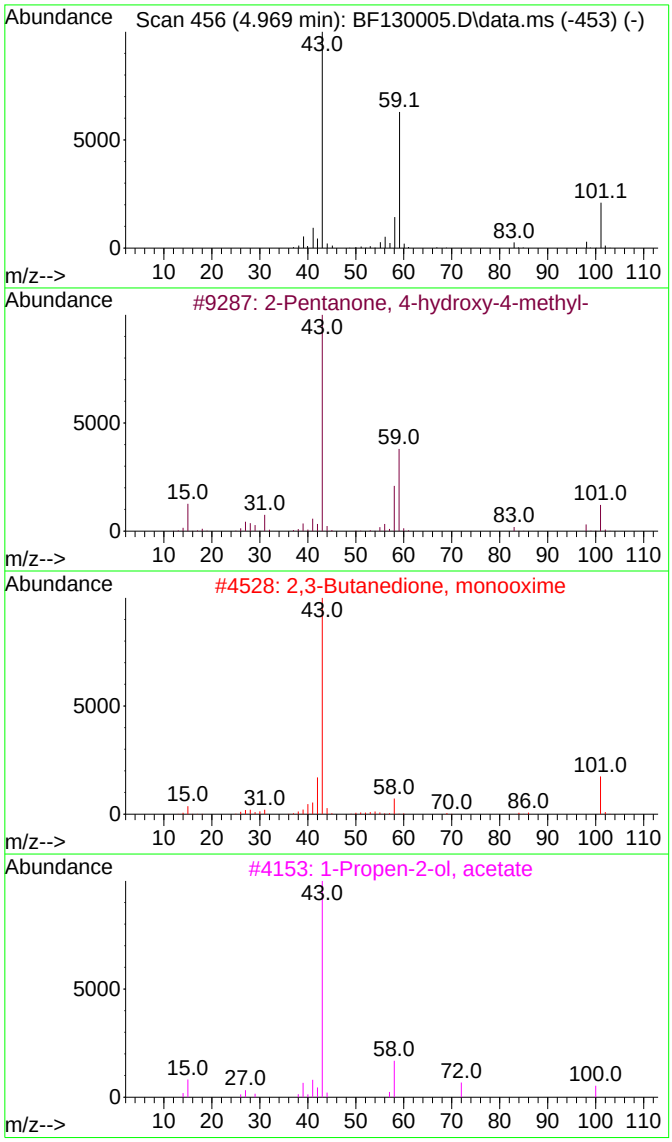
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

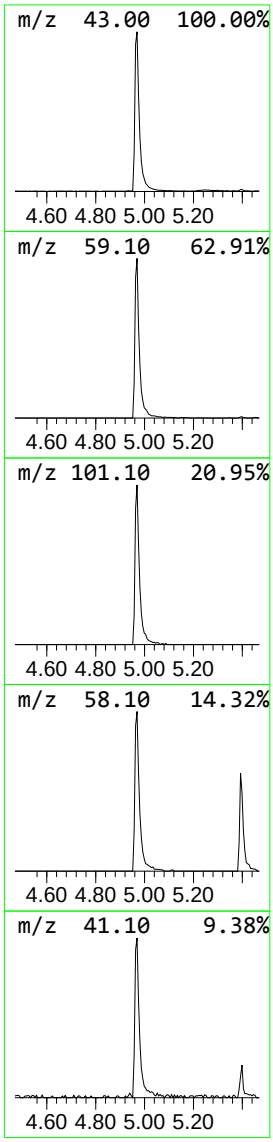
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.969	15.85 ng	504172	1,4-Dichlorobenzene-d4	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9





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Data File : BF130005.D
Acq On : 25 Aug 2022 18:19
Operator : CG\JU
Sample : N4352-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
11985

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

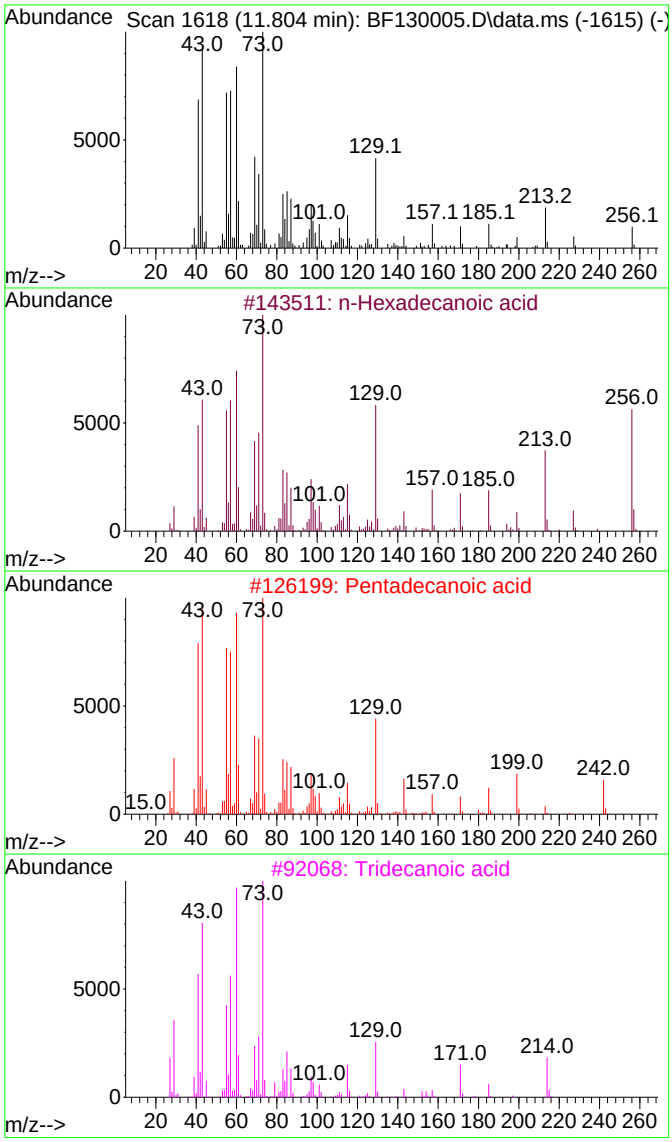
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

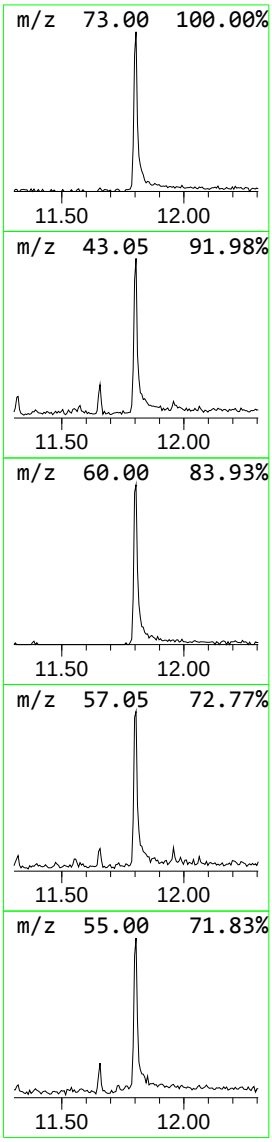
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	7.00 ng	230395	Phenanthrene-d10	11.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF130005.D
Acq On : 25 Aug 2022 18:19
Operator : CG\JU
Sample : N4352-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
11985

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

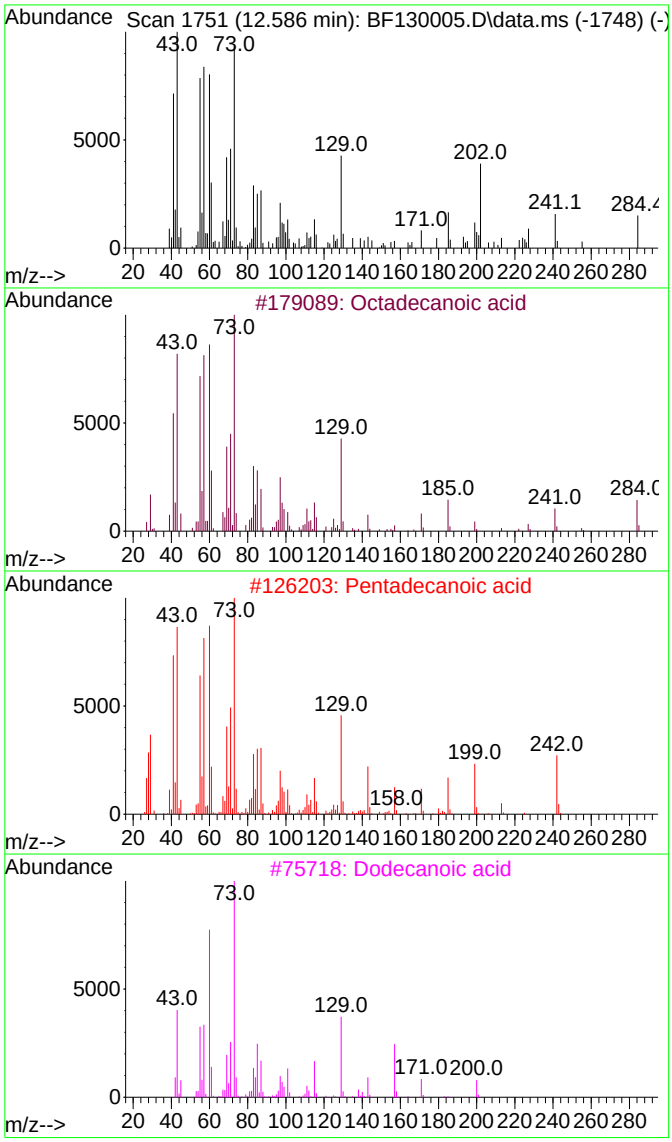
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

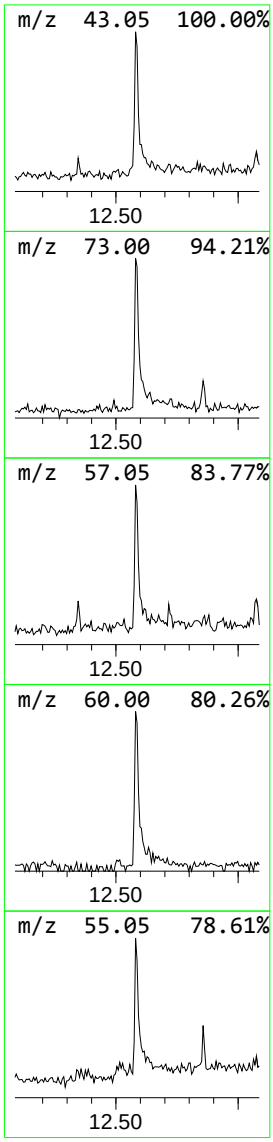
****

Peak Number 3 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.586	3.08 ng	101286	Phenanthrene-d10	11.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	Hexadecane	226	C16H34	000544-76-3	56
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF130005.D
Acq On : 25 Aug 2022 18:19
Operator : CG\JU
Sample : N4352-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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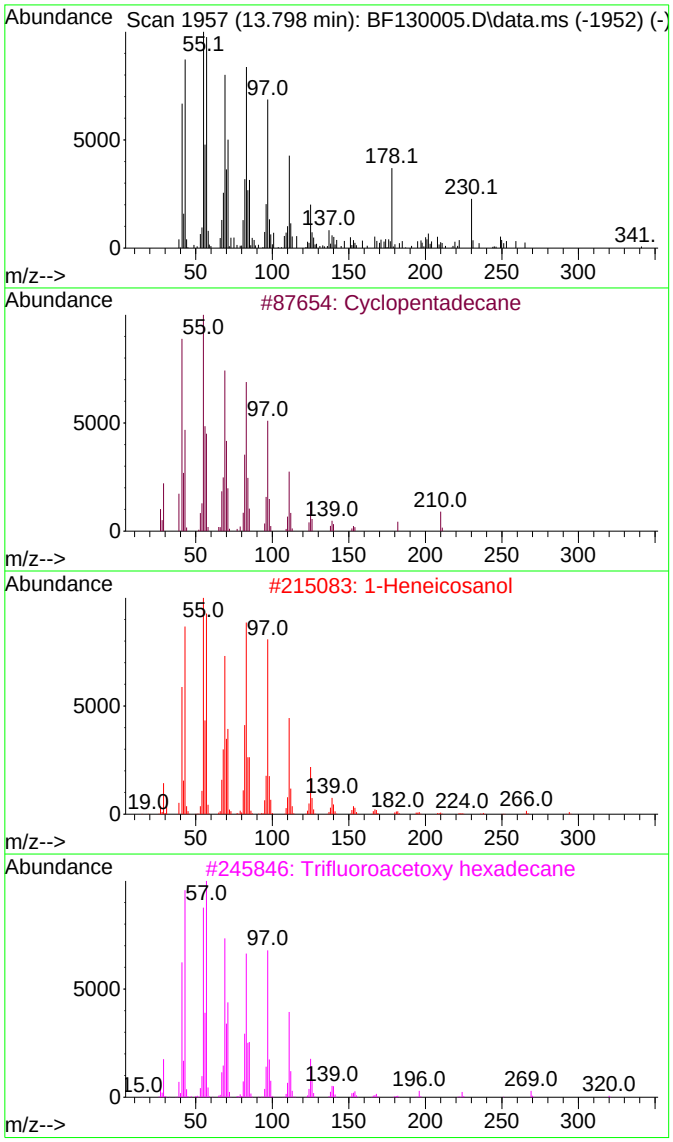
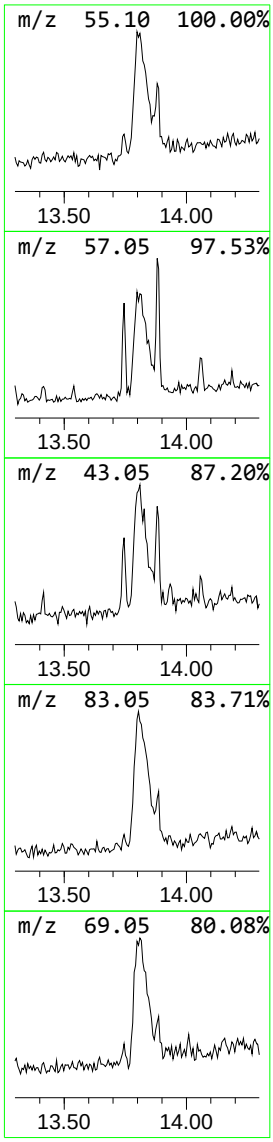
Peak Number 4 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	6.50 ng	307360	Chrysene-d12	13.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	1-Hexacosene	364	C26H52	018835-33-1	91
5	Behenic alcohol	326	C22H46O	000661-19-8	87





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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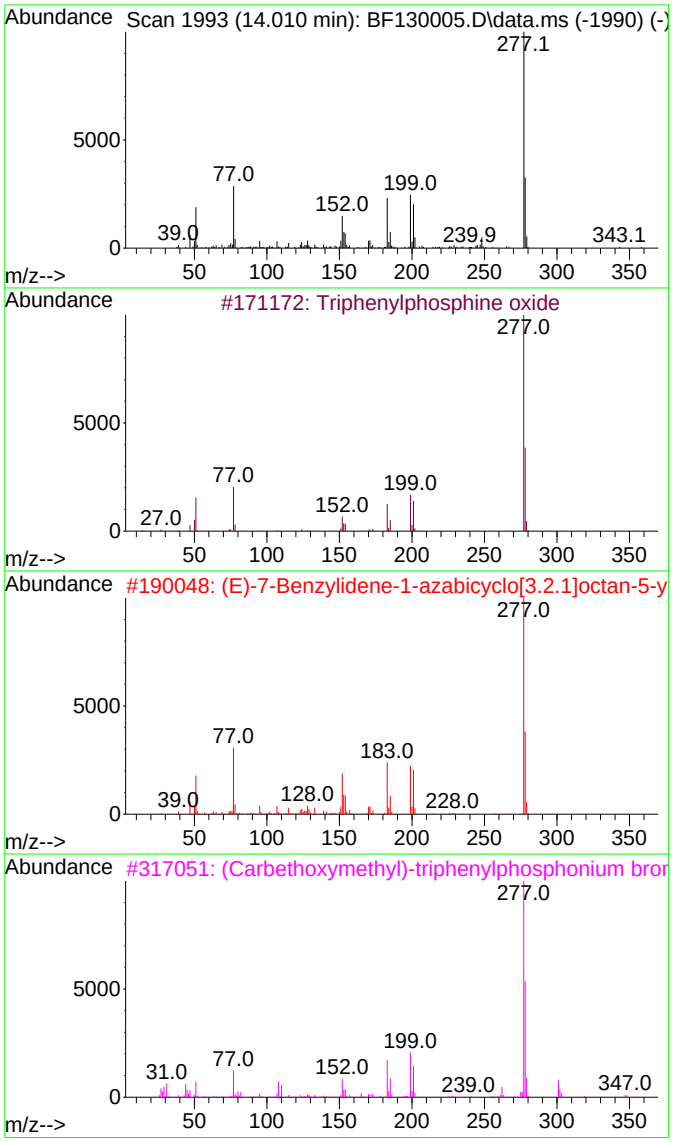
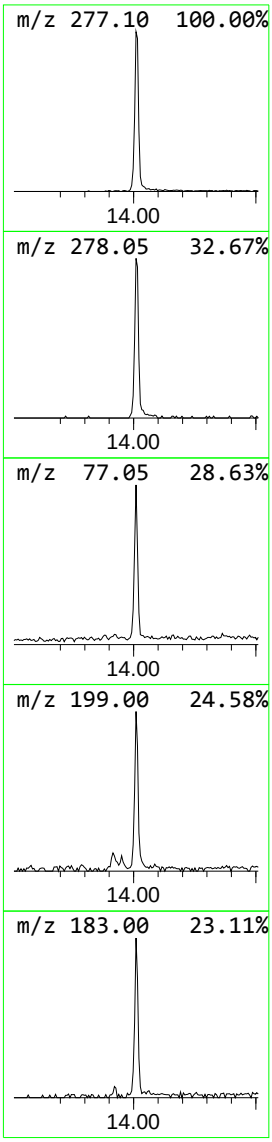
Peak Number 5 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.010	4.18 ng	197771	Chrysene-d12	13.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	47
4	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	38
5	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	38





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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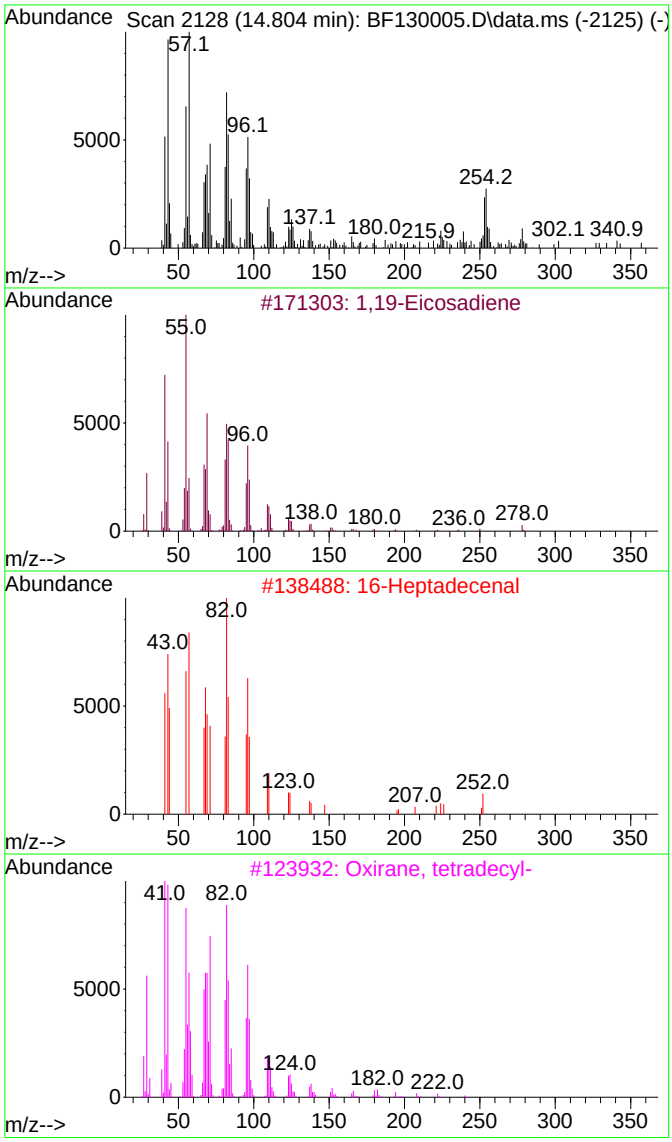
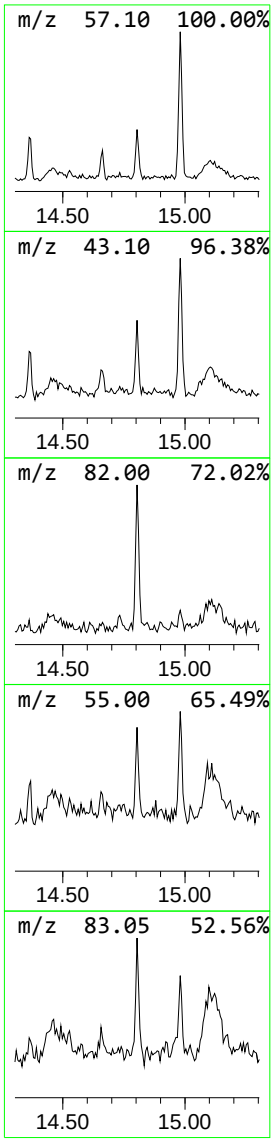
Peak Number 6 1,19-Eicosadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	3.50 ng	115377	Perylene-d12	15.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	92
2	16-Heptadecenal	252	C17H32O	1010144-57-9	92
3	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	90
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	89
5	Octadecanal	268	C18H36O	000638-66-4	89





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

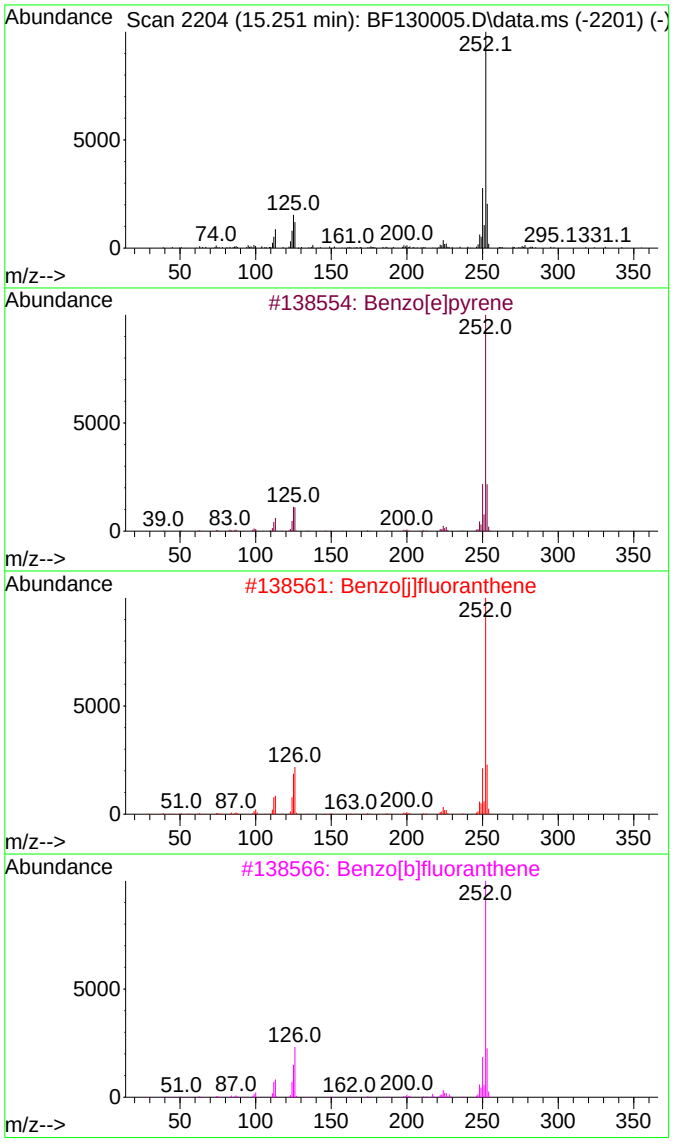
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

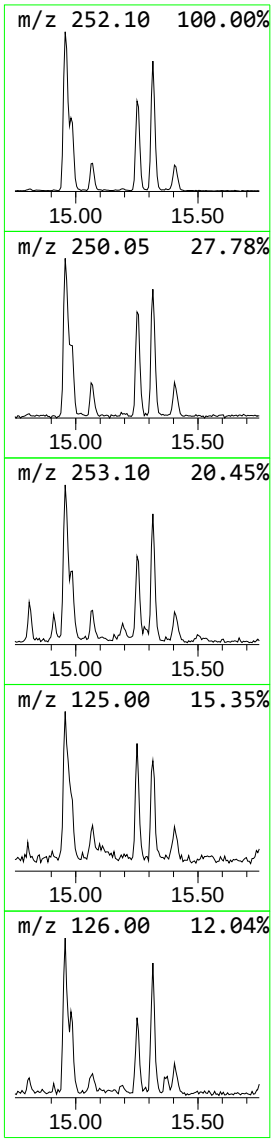
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.251	4.25 ng	140201	Perylene-d12	15.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Perylene	252	C20H12	000198-55-0	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF130005.D
Acq On : 25 Aug 2022 18:19
Operator : CG\JU
Sample : N4352-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
11985

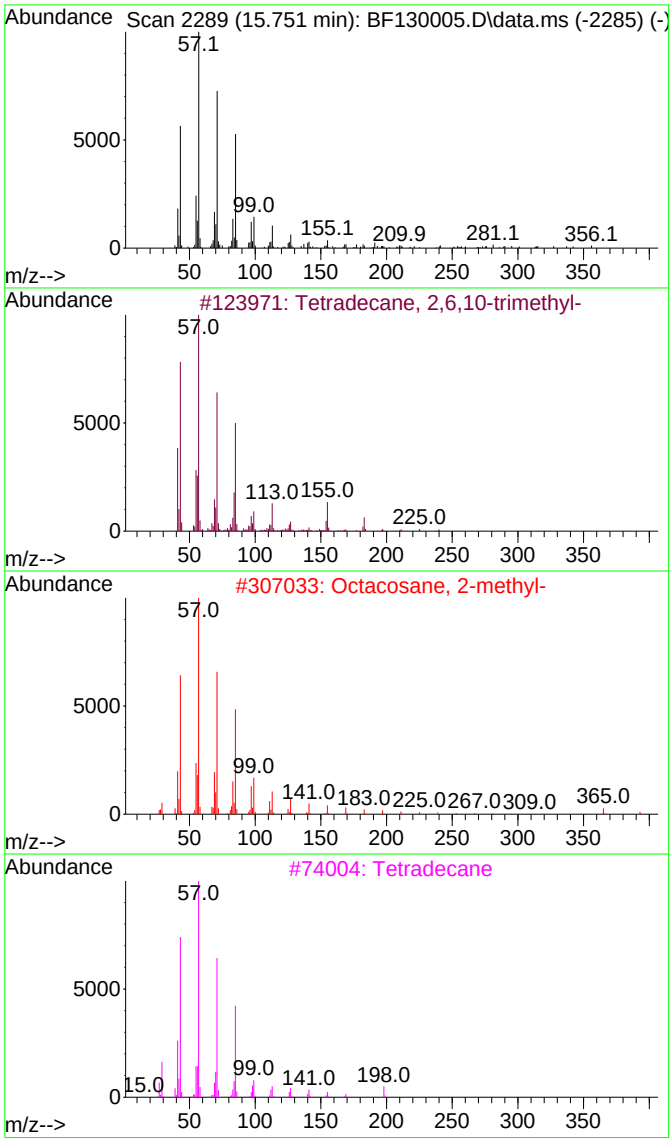
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

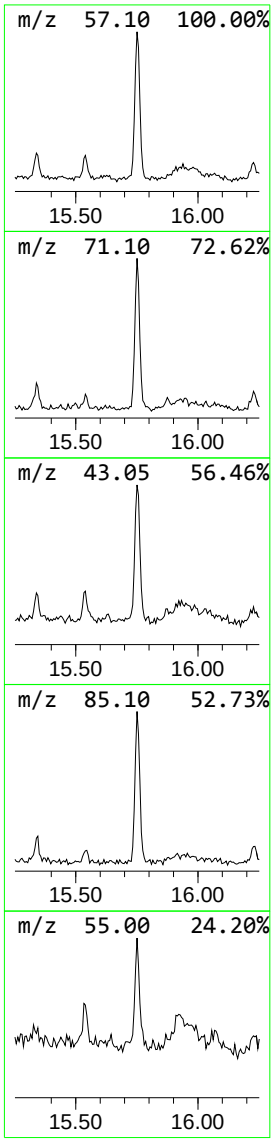
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Tetradecane, 2,6,10-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	5.55 ng	183048	Perylene-d12	15.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3	Tetradecane	198	C14H30	000629-59-4	83
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	83
5	Hexadecane, 7-methyl-	240	C17H36	026730-20-1	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF130005.D
Acq On : 25 Aug 2022 18:19
Operator : CG\JU
Sample : N4352-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
11985

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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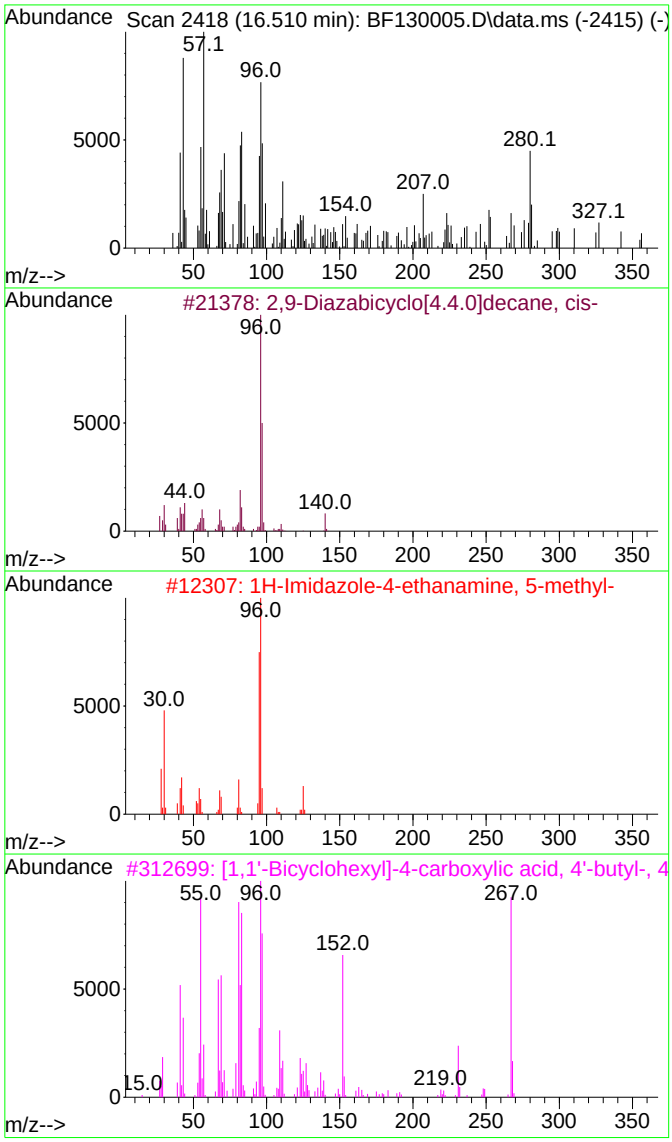
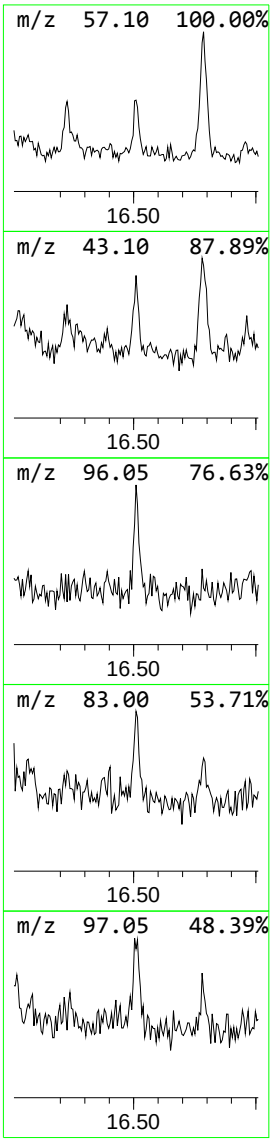
Peak Number 9 unknown16.510 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.510	2.22 ng	73119	Perylene-d12	15.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,9-Diazabicyclo[4.4.0]decane, cis-	140	C8H16N2	093955-52-3	35
2	1H-Imidazole-4-ethanamine, 5-met...	125	C6H11N3	036507-31-0	35
3	[1,1'-Bicyclohexyl]-4-carboxylic...	418	C28H50O2	102714-86-3	32
4	3-Dimethylaminoacrylonitrile	96	C5H8N2	002407-68-3	25
5	Carbonic acid, butyl cyclohexylm...	214	C12H22O3	1010357-84-5	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF130005.D
Acq On : 25 Aug 2022 18:19
Operator : CG\JU
Sample : N4352-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
11985

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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
2-Pentanone, 4-...	4.969	15.9	ng	504172	1	6.757	635986	20.0
n-Hexadecanoic ...	11.804	7.0	ng	230395	4	11.275	658394	20.0
Octadecanoic acid	12.586	3.1	ng	101286	4	11.275	658394	20.0
Cyclopentadecane	13.798	6.5	ng	307360	5	13.927	945315	20.0
Triphenylphosph...	14.010	4.2	ng	197771	5	13.927	945315	20.0
1,19-Eicosadiene	14.804	3.5	ng	115377	6	15.374	660029	20.0
Benzo[e]pyrene	15.251	4.3	ng	140201	6	15.374	660029	20.0
Tetradecane, 2,...	15.751	5.5	ng	183048	6	15.374	660029	20.0
unknown16.510	16.510	2.2	ng	73119	6	15.374	660029	20.0