LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130942.D
Acq On : 02 Nov 2022 21:41
Operator : CG\JU
Sample : N5395-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-9-103122

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130942.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	15	23	31	rVB	439752	577505	36.12%	4.589%
2	2.334	37	42	48	rVB	31581	40773	2.55%	0.324%
3	4.034	325	331	336	rVB	150827	192934	12.07%	1.533%
4	5.145	516	520	530	rBV	337303	399249	24.97%	3.172%
5	5.540	582	587	590	rBV	1772061	1581518	98.91%	12.567%
6	6.539	752	757	771	rVB	1465152	1598930	100.00%	12.705%
7	6.922	818	822	826	rBV	498878	384675	24.06%	3.057%
8	7.316	886	889	902	rBV	93840	90126	5.64%	0.716%
9	7.486	913	918	921	rBV	1122908	988184	61.80%	7.852%
10	8.116	1020	1025	1033	rBV2	24018	61003	3.82%	0.485%
11	8.210	1037	1041	1043	rVV	500370	468010	29.27%	3.719%
12	8.228	1043	1044	1047	rVB	38117	21703	1.36%	0.172%
13	9.286	1219	1224	1227	rBV	1538867	1412669	88.35%	11.225%
14	9.969	1336	1340	1343	rVB	536745	429906	26.89%	3.416%
15	10.757	1470	1474	1477	rBV	891730	723606	45.26%	5.750%
16	10.804	1479	1482	1485	rVB	32801	25768	1.61%	0.205%
17	10.880	1491	1495	1502	rVB2	16453	24271	1.52%	0.193%
18	11.457	1590	1593	1596	rBV	410478	358736	22.44%	2.851%
19	11.480	1596	1597	1600	rVV	83063	57929	3.62%	0.460%
20	11.533	1602	1606	1608	rVB2	16653	18848	1.18%	0.150%
21	11.974	1676	1681	1688	rBV3	30035	49565	3.10%	0.394%
22	12.074	1694	1698	1700	rBV2	19876	20649	1.29%	0.164%
23	12.674	1797	1800	1804	rBV	161608	130693	8.17%	1.039%
24	12.904	1834	1839	1843	rBV	118628	136697	8.55%	1.086%
25	13.051	1860	1864	1867	rVB	1065764	956031	59.79%	7.597%
26	13.121	1872	1876	1881	rBV5	12394	25037	1.57%	0.199%
27	13.186	1883	1887	1889	rBV	18460	19841	1.24%	0.158%
28	13.233	1892	1895	1899	rVB	27721	27596	1.73%	0.219%
29	13.274	1899	1902	1904	rBV2	15751	16973	1.06%	0.135%
30	13.304	1904	1907	1909	rBV	20698	18027	1.13%	0.143%
31	13.945	2014	2016	2023	rVB3	33696	32623	2.04%	0.259%
32	14.027	2025	2030	2033	rBV6	35465	75055	4.69%	0.596%
33	14.110	2039	2044	2046	rBV2	406681	417382	26.10%	3.317%
34	14.133	2046	2048	2055	rVB	94820	85451	5.34%	0.679%
35	14.568	2120	2122	2128	rVB3	31644	35751	2.24%	0.284%
36	15.168	2220	2224	2228	rBV	78515	132251	8.27%	1.051%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130942.D
Acq On : 02 Nov 2022 21:41
Operator : CG\JU
Sample : N5395-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-9-103122

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.245	2234	2237	2241	rVB2	49142	54675	3.42%	0.434%
38	15.486	2275	2278	2285	rVB	52203	76361	4.78%	0.607%
39	15.551	2285	2289	2295	rBV	69304	90345	5.65%	0.718%
40	15.621	2296	2301	2304	rBV	311093	389741	24.38%	3.097%
41	16.109	2380	2384	2391	rVB	55366	87320	5.46%	0.694%
42	16.362	2422	2427	2428	rBV5	21095	33529	2.10%	0.266%
43	16.962	2525	2529	2538	rVB5	20151	44038	2.75%	0.350%
44	17.145	2557	2560	2568	rVB3	29432	53661	3.36%	0.426%
45	17.280	2577	2583	2589	rVB2	55804	119088	7.45%	0.946%

Sum of corrected areas: 12584723

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
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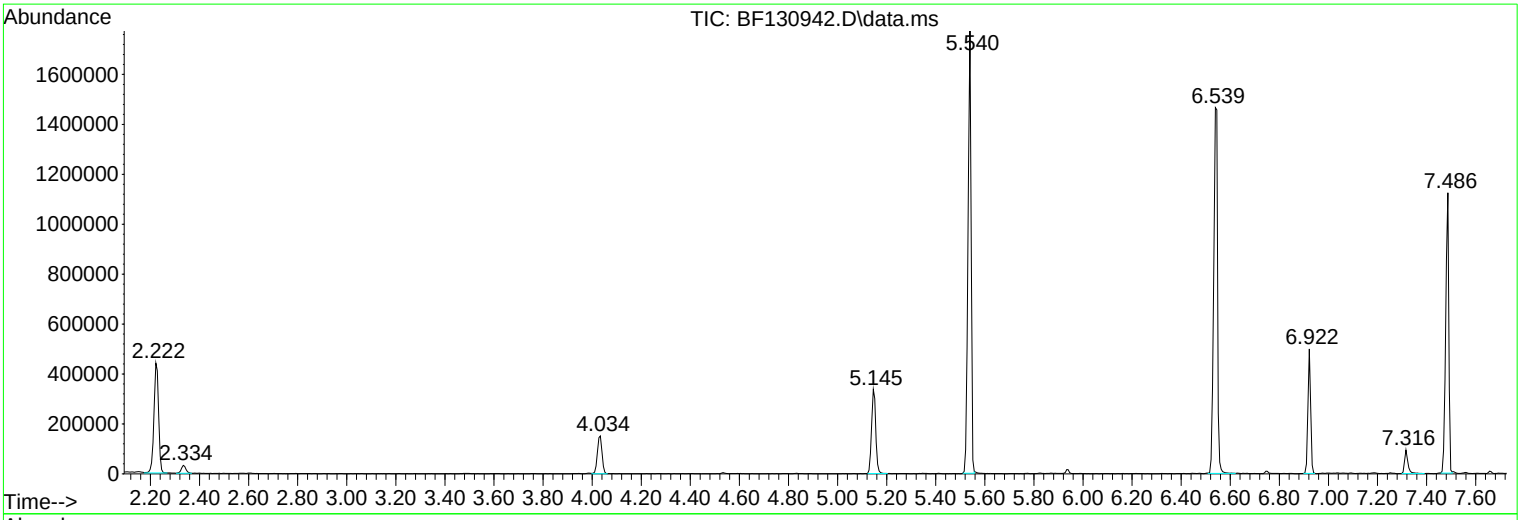
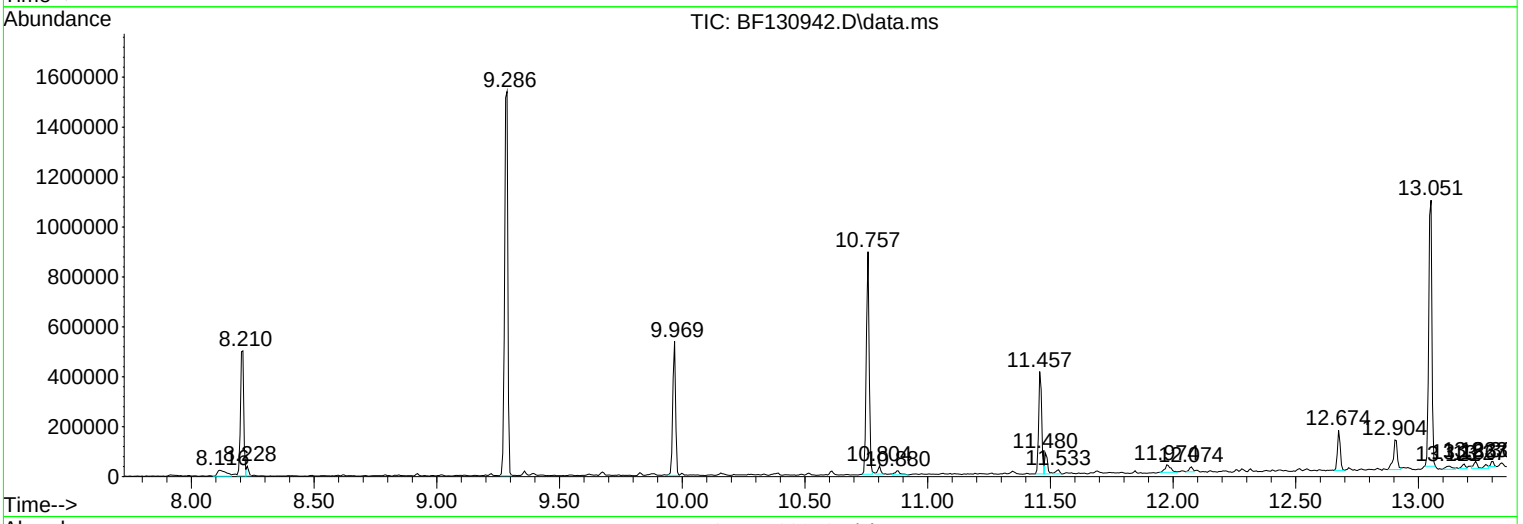
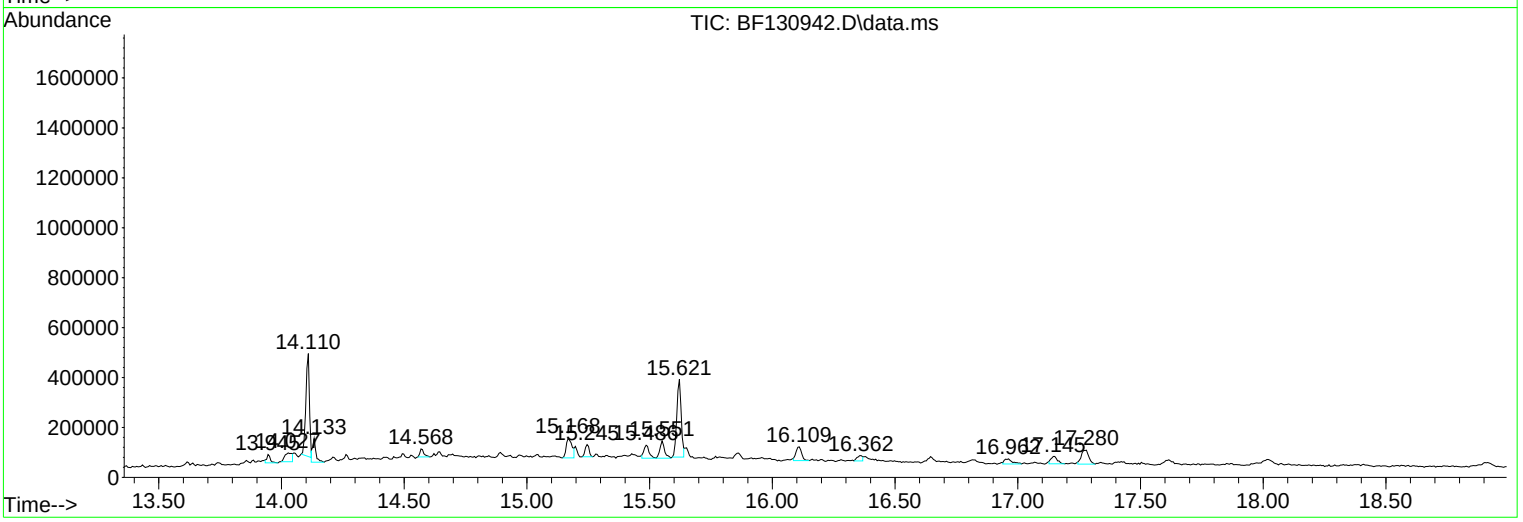
Instrument :
BNA_F
ClientSampleId :
S-9-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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\BF110222\
Data File : BF130942.D
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Operator : CG\JU
Sample : N5395-12
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Instrument :
BNA_F
ClientSampleId :
S-9-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

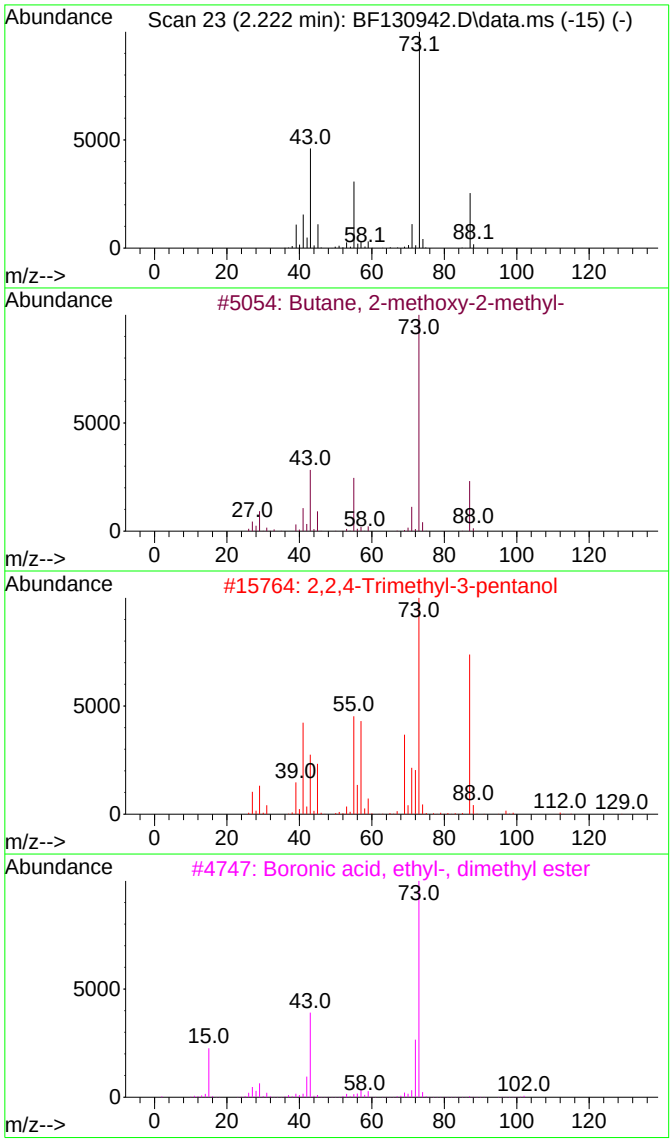
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

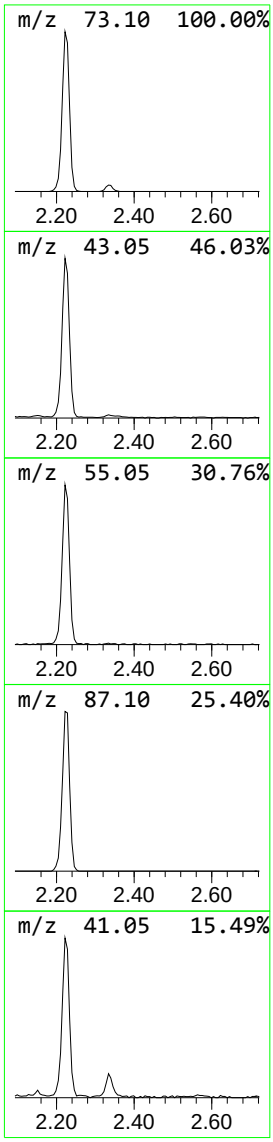
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	30.03 ng	577505	1,4-Dichlorobenzene-d4	6.922

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	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Instrument :
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ClientSampleId :
S-9-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

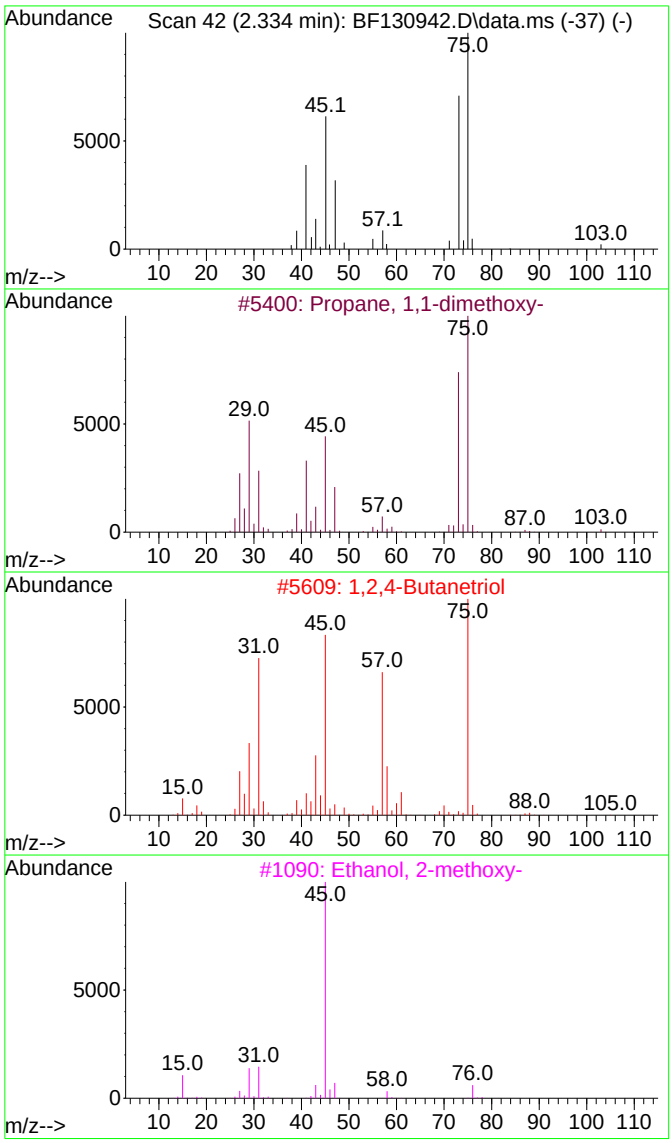
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

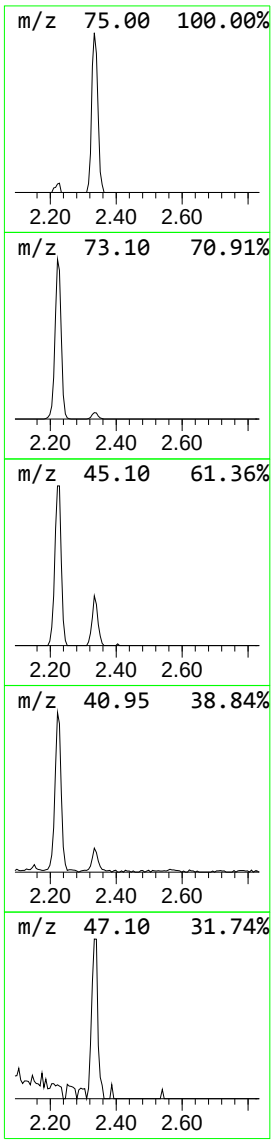
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.334	2.12 ng	40773	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	1,2,4-Butanetriol	106	C4H10O3	003068-00-6	38
3	Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	10
4	2-Hydrazinoethanol	76	C2H8N2O	000109-84-2	9
5	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130942.D
Acq On : 02 Nov 2022 21:41
Operator : CG\JU
Sample : N5395-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-9-103122

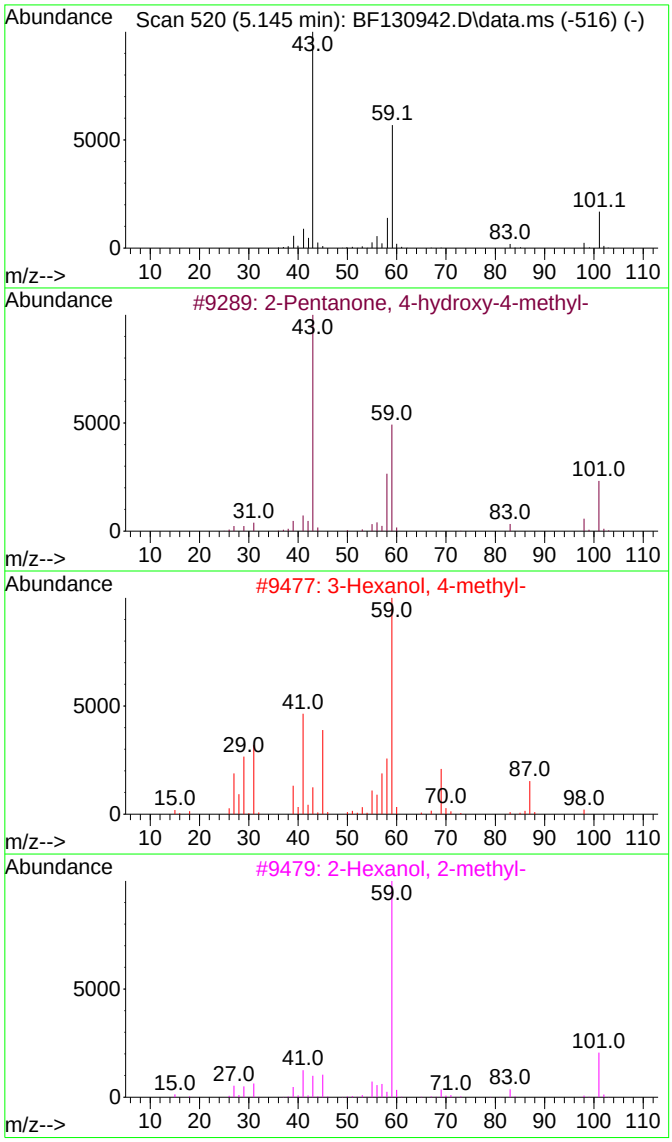
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

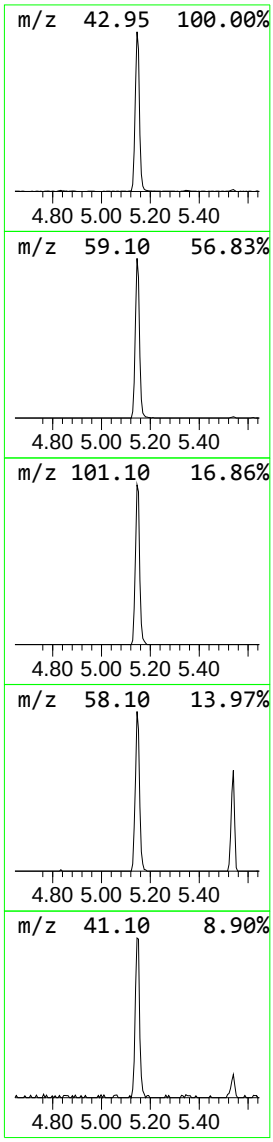
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.145	20.76 ng	399249	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Instrument :
BNA_F
ClientSampleId :
S-9-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

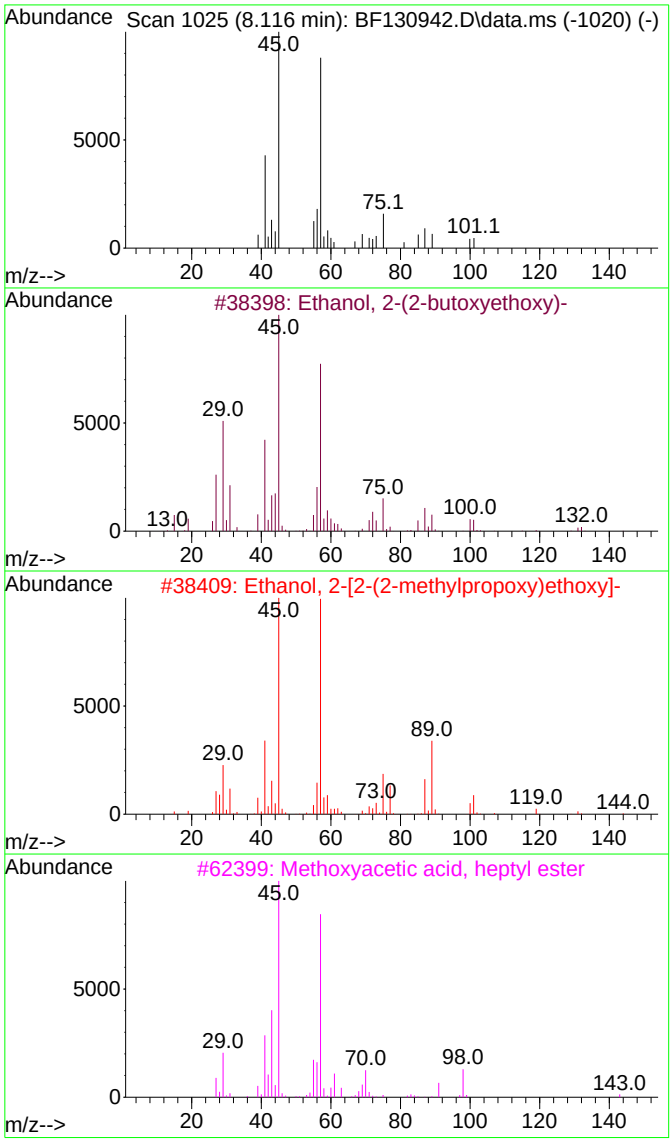
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

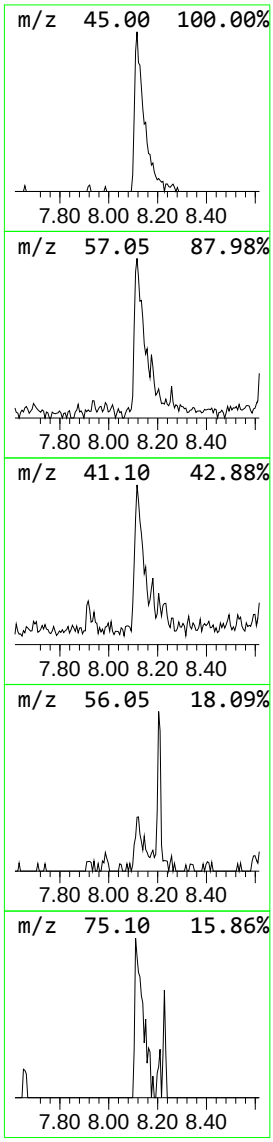
****

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.116	2.61 ng	61003	Naphthalene-d8	8.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50
4	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	42
5	2-Hexanol, 5-methyl-	116	C7H16O	000627-59-8	38





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Data File : BF130942.D
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Operator : CG\JU
Sample : N5395-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-9-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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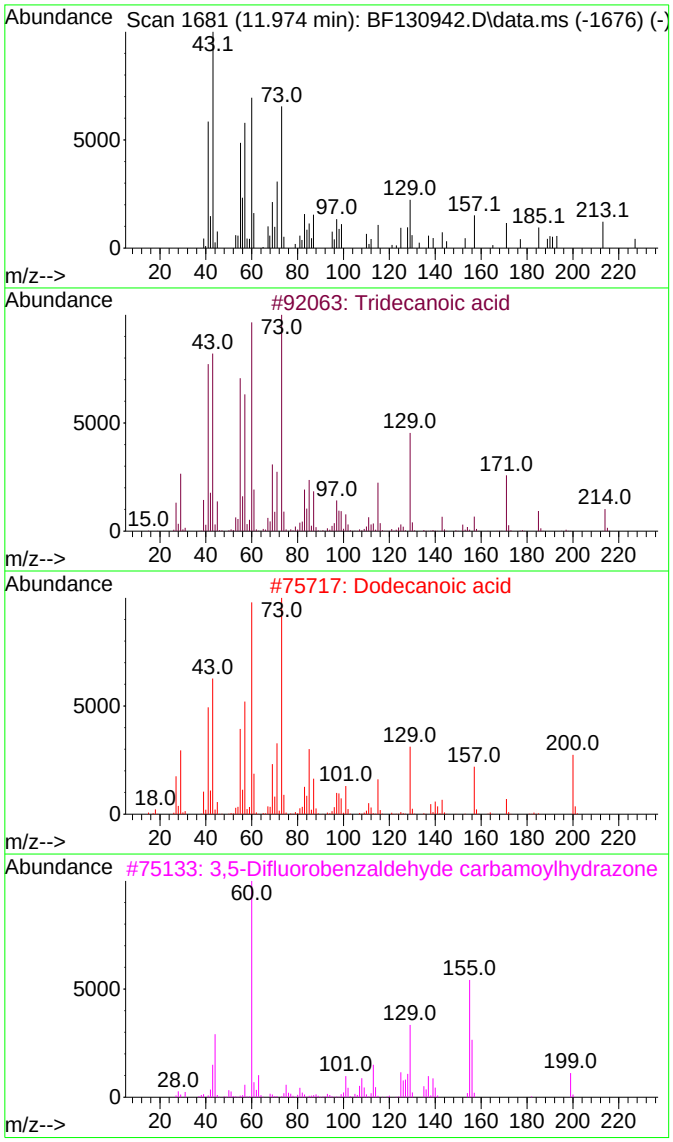
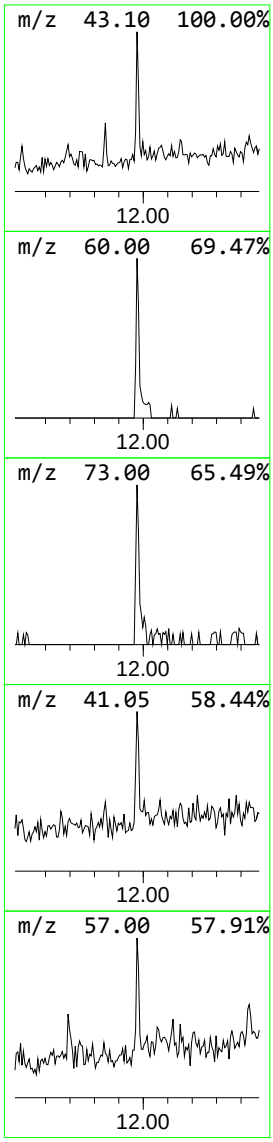
Peak Number 6 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.974	2.76 ng	49565	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	52
2	Dodecanoic acid	200	C12H24O2	000143-07-7	49
3	3,5-Difluorobenzaldehyde carbamo...	199	C8H7F2N3O	163893-49-0	43
4	Undecanoic acid	186	C11H22O2	000112-37-8	35
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	35





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Sample : N5395-12
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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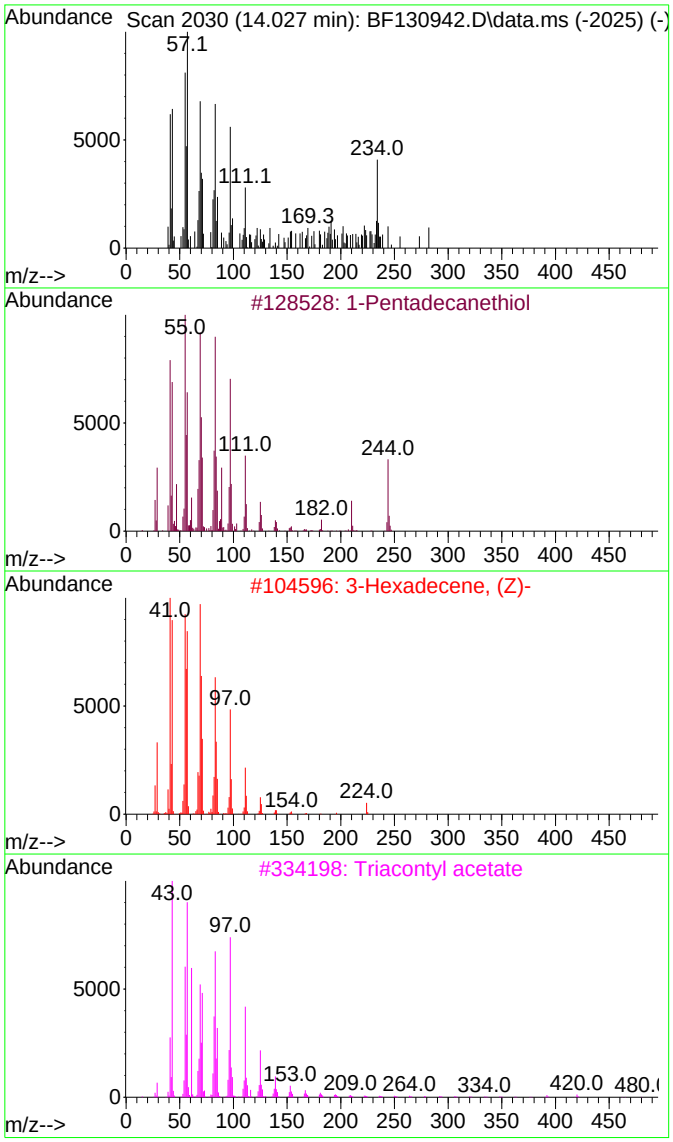
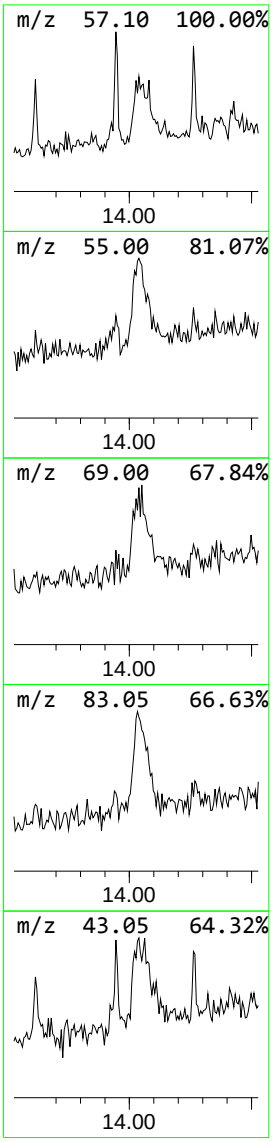
Peak Number 7 1-Pentadecanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.027	3.60 ng	75055	Chrysene-d12	14.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecanethiol	244	C15H32S	025276-70-4	55
2	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	47
3	Triacontyl acetate	480	C32H64O2	041755-58-2	46
4	Cyclohexadecane	224	C16H32	000295-65-8	45
5	1-Dodecene	168	C12H24	000112-41-4	41





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Instrument :
BNA_F
ClientSampleId :
S-9-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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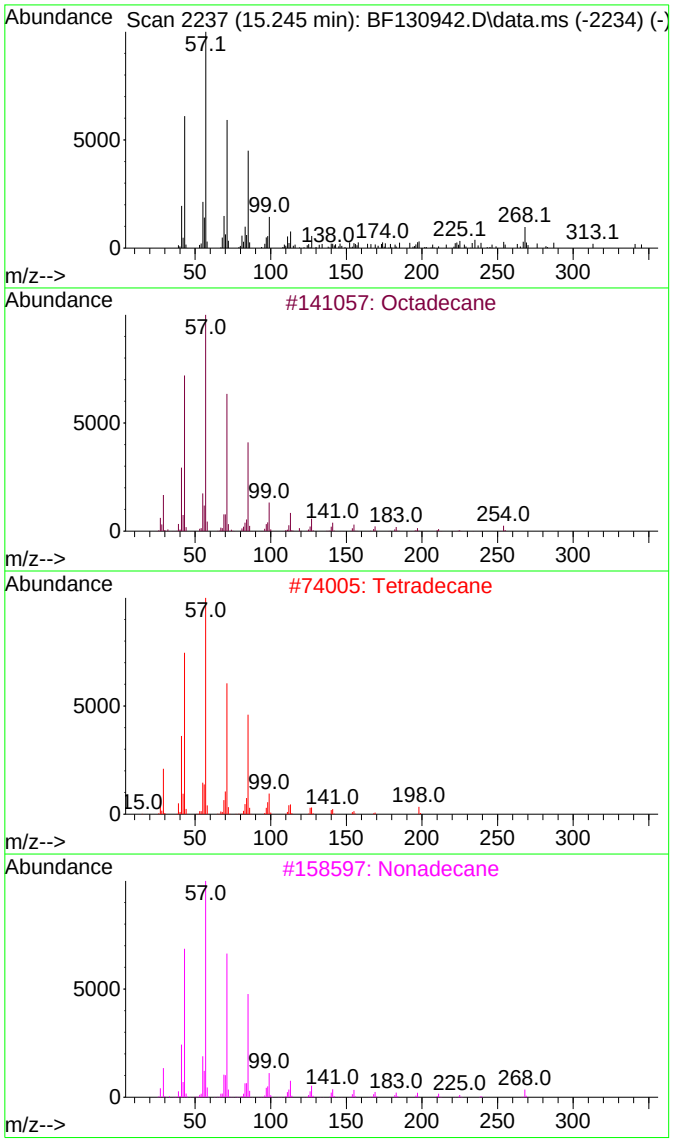
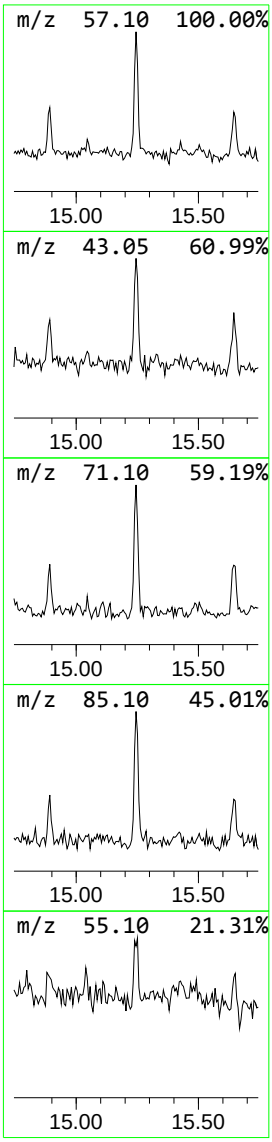
Peak Number 8 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	2.81 ng	54675	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Tetradecane	198	C14H30	000629-59-4	90
3	Nonadecane	268	C19H40	000629-92-5	87
4	Heptacosane	380	C27H56	000593-49-7	74
5	Octacosane	394	C28H58	000630-02-4	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130942.D
Acq On : 02 Nov 2022 21:41
Operator : CG\JU
Sample : N5395-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-9-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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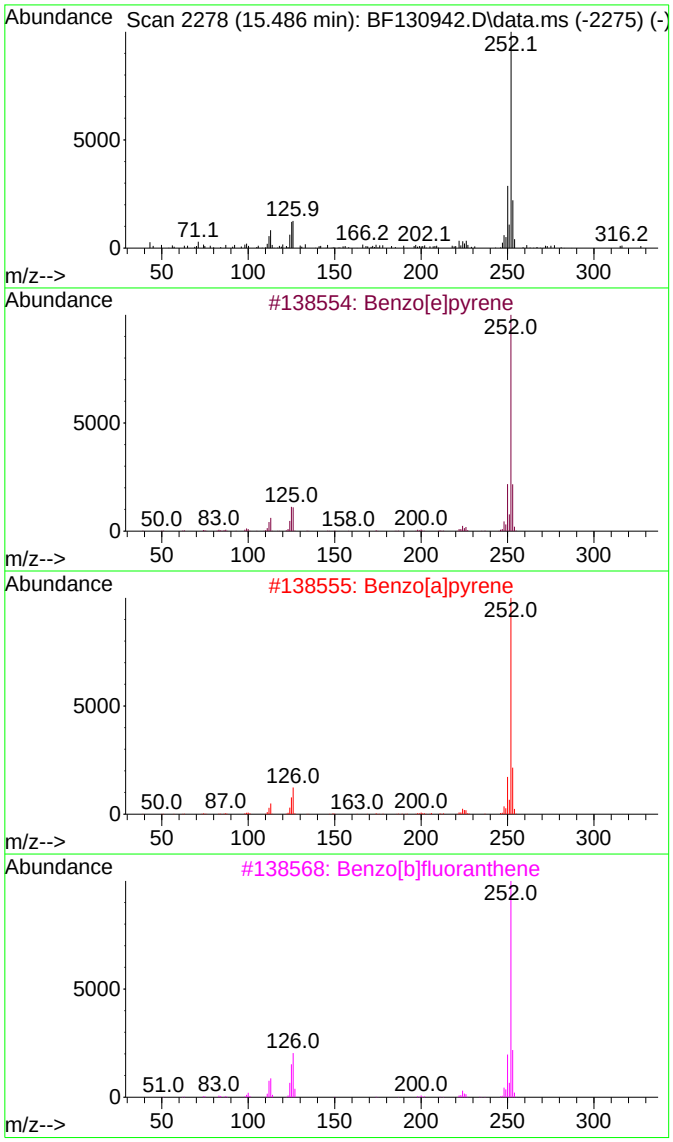
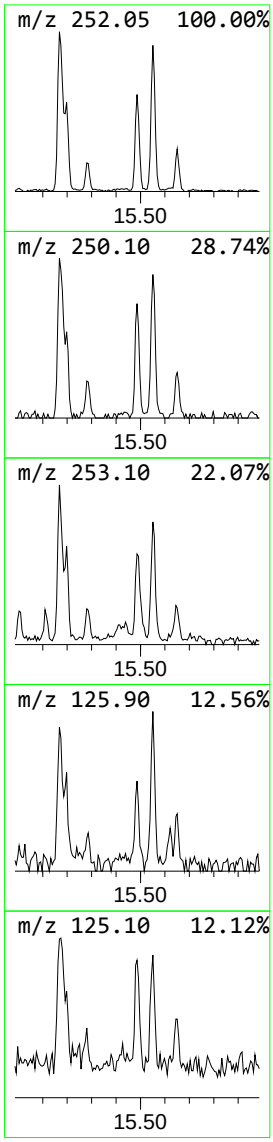
Peak Number 9 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.486	3.92 ng	76361	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
4	Perylene	252	C20H12	000198-55-0	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91





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Acq On : 02 Nov 2022 21:41
Operator : CG\JU
Sample : N5395-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-9-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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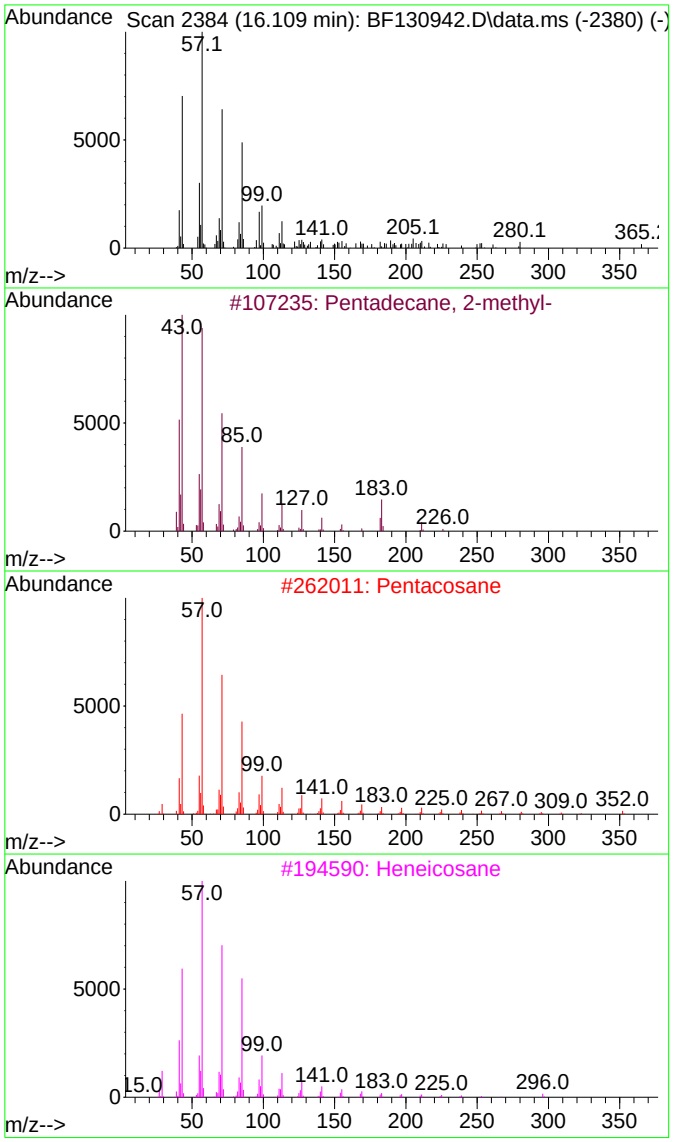
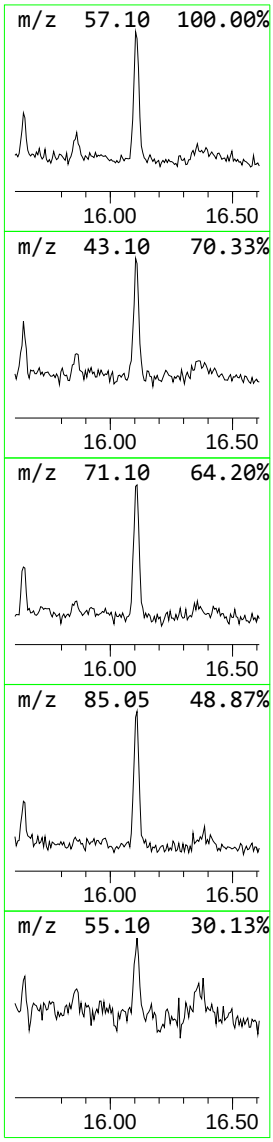
Peak Number 10 Pentadecane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.109	4.48 ng	87320	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	86
2	Pentacosane	352	C25H52	000629-99-2	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	80
5	Hexadecane	226	C16H34	000544-76-3	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130942.D
Acq On : 02 Nov 2022 21:41
Operator : CG\JU
Sample : N5395-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-9-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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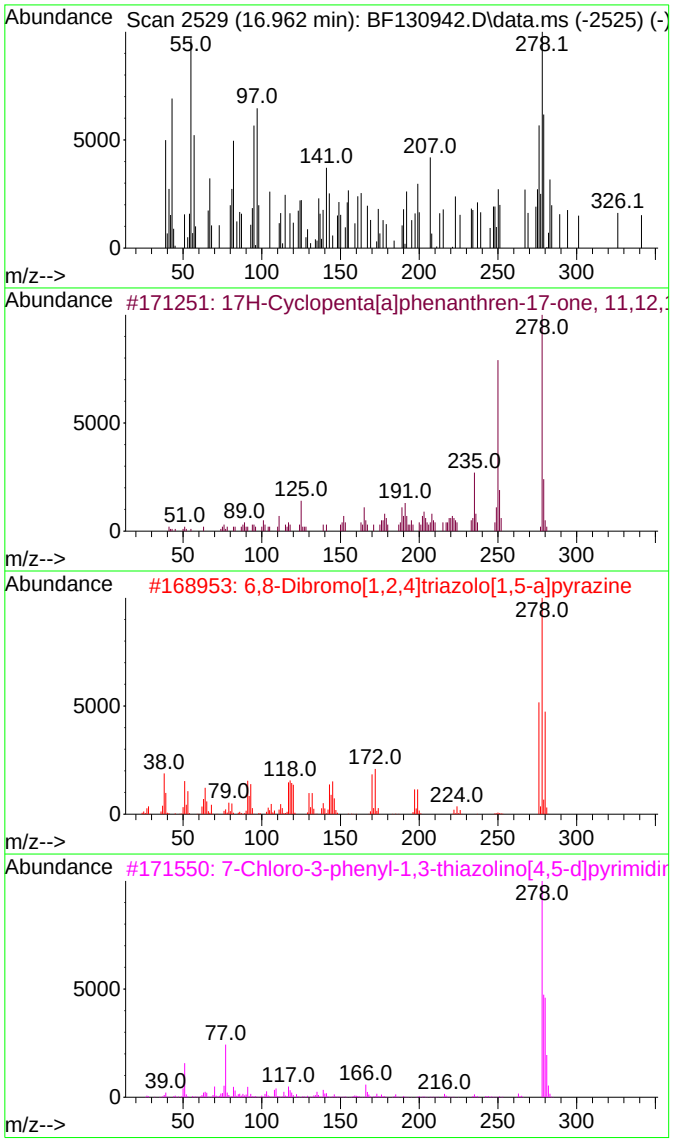
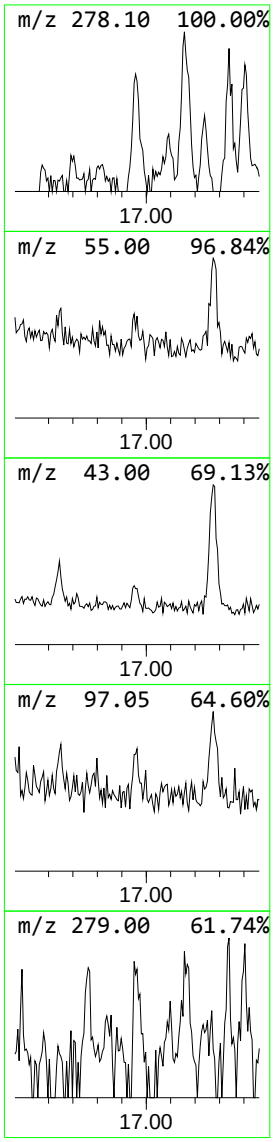
Peak Number 11 unknown16.962 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.962	2.26 ng	44038	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17H-Cyclopenta[a]phenanthren-17-...	278	C19H18O2	056614-59-6	27
2	6,8-Dibromo[1,2,4]triazolo[1,5-a...	276	C5H2Br2N4	944709-42-6	27
3	7-Chloro-3-phenyl-1,3-thiazolino...	279	C11H6ClN3S2	189766-33-4	27
4	Anthraquinone, 2,6-dichloro-	276	C14H6Cl2O2	000605-40-3	22
5	1,2,3,4-Phenazinetetrol, 7-chloro-	278	C12H7ClN2O4	023774-10-9	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130942.D
Acq On : 02 Nov 2022 21:41
Operator : CG\JU
Sample : N5395-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-9-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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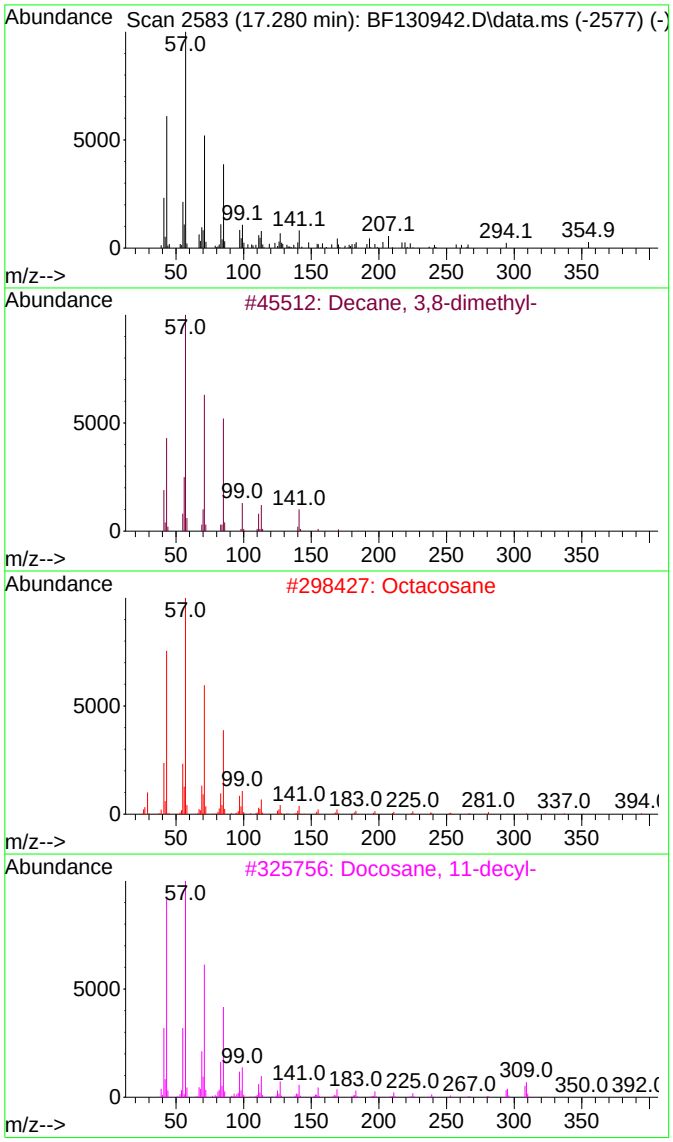
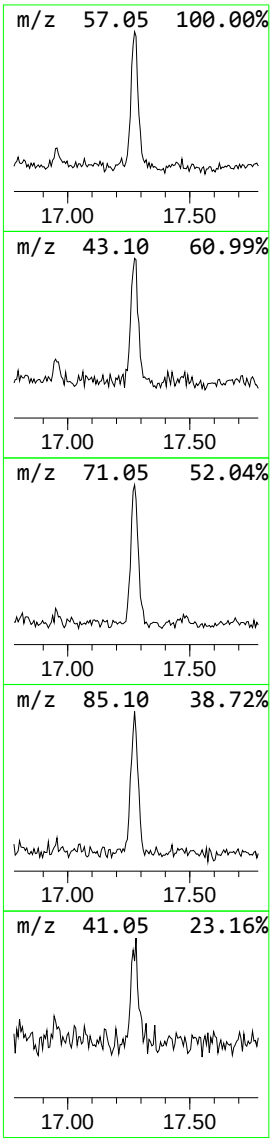
Peak Number 12 Decane, 3,8-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.280	6.11 ng	119088	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	83
2	Octacosane	394	C28H58	000630-02-4	83
3	Docosane, 11-decyl-	451	C32H66	055401-55-3	83
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	83
5	Hentriacontane	437	C31H64	000630-04-6	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130942.D
Acq On : 02 Nov 2022 21:41
Operator : CG\JU
Sample : N5395-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-9-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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
Butane, 2-metho...	2.222	30.0	ng	577505	1	6.922	384675	20.0
Propane, 1,1-di...	2.334	2.1	ng	40773	1	6.922	384675	20.0
2-Pentanone, 4-...	5.145	20.8	ng	399249	1	6.922	384675	20.0
Ethanol, 2-(2-b...	8.116	2.6	ng	61003	2	8.210	468010	20.0
Tridecanoic acid	11.974	2.8	ng	49565	4	11.457	358736	20.0
1-Pentadecanethiol	14.027	3.6	ng	75055	5	14.110	417382	20.0
Octadecane	15.245	2.8	ng	54675	6	15.621	389741	20.0
Benzo[e]pyrene	15.486	3.9	ng	76361	6	15.621	389741	20.0
Pentadecane, 2-...	16.109	4.5	ng	87320	6	15.621	389741	20.0
unknown16.962	16.962	2.3	ng	44038	6	15.621	389741	20.0
Decane, 3,8-dim...	17.280	6.1	ng	119088	6	15.621	389741	20.0