LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130945.D
Acq On : 02 Nov 2022 23:19
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-4-103122

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: BF130945.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	16	24	30	rVB	488523	627364	38.64%	5.006%
2	2.340	38	43	53	rVB	31994	44887	2.76%	0.358%
3	4.034	326	331	337	rVB	131029	156419	9.63%	1.248%
4	5.151	516	521	532	rVB	333847	401745	24.74%	3.206%
5	5.539	582	587	590	rBV	1713102	1623816	100.00%	12.957%
6	5.939	651	655	660	rVB	16988	17204	1.06%	0.137%
7	6.545	752	758	765	rVB	1513421	1581556	97.40%	12.620%
8	6.751	789	793	797	rBV3	13979	16623	1.02%	0.133%
9	6.922	819	822	825	rBV	513421	385400	23.73%	3.075%
10	7.063	843	846	851	rBV3	16708	25210	1.55%	0.201%
11	7.316	886	889	898	rVB	60838	60872	3.75%	0.486%
12	7.486	913	918	921	rBV	1151460	972886	59.91%	7.763%
13	8.110	1020	1024	1037	rBV	77944	184807	11.38%	1.475%
14	8.210	1037	1041	1043	rVV	487998	446283	27.48%	3.561%
15	8.228	1043	1044	1048	rVB	31356	19401	1.19%	0.155%
16	9.280	1219	1223	1227	rBV	1360298	1212679	74.68%	9.676%
17	9.969	1336	1340	1343	rVB	488741	386586	23.81%	3.085%
18	10.610	1446	1449	1453	rBV2	25954	22122	1.36%	0.177%
19	10.757	1470	1474	1477	rBV	902308	734460	45.23%	5.861%
20	10.804	1479	1482	1488	rVV	52976	50355	3.10%	0.402%
21	10.880	1490	1495	1502	rVB3	17341	28322	1.74%	0.226%
22	11.457	1590	1593	1596	rBV	380093	349068	21.50%	2.785%
23	11.480	1596	1597	1600	rVV	76103	55348	3.41%	0.442%
24	11.533	1602	1606	1609	rVB	19073	18408	1.13%	0.147%
25	11.845	1656	1659	1662	rBV	26687	21299	1.31%	0.170%
26	11.974	1676	1681	1690	rBV4	27265	53303	3.28%	0.425%
27	12.074	1695	1698	1701	rBV	19859	20548	1.27%	0.164%
28	12.551	1775	1779	1782	rBV6	12612	16919	1.04%	0.135%
29	12.674	1797	1800	1804	rVB	183527	154036	9.49%	1.229%
30	12.910	1834	1840	1843	rBV	142682	166636	10.26%	1.330%
31	13.051	1860	1864	1867	rVB	1159274	977510	60.20%	7.800%
32	13.127	1872	1877	1880	rBV5	12707	24903	1.53%	0.199%
33	13.233	1892	1895	1898	rVB	29425	26174	1.61%	0.209%
34	13.304	1904	1907	1909	rBV	19238	16518	1.02%	0.132%
35	13.339	1910	1913	1916	rBV3	16725	18440	1.14%	0.147%
36	13.945	2014	2016	2020	rVB3	35502	34417	2.12%	0.275%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130945.D
Acq On : 02 Nov 2022 23:19
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-103122

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	14.033	2025	2031	2032	rBV4	36710	67124	4.13%	0.536%
38	14.109	2039	2044	2046	rBV2	483188	477521	29.41%	3.810%
39	14.133	2046	2048	2053	rVB	102410	91762	5.65%	0.732%
40	14.574	2120	2123	2128	rVB4	32227	36778	2.26%	0.293%
41	14.645	2133	2135	2139	rVB4	24741	21510	1.32%	0.172%
42	14.892	2175	2177	2180	rVB2	26047	19985	1.23%	0.159%
43	15.168	2221	2224	2228	rBV	75462	123985	7.64%	0.989%
44	15.245	2234	2237	2241	rVB	57578	61733	3.80%	0.493%
45	15.486	2276	2278	2285	rVB	50176	65080	4.01%	0.519%
46	15.551	2286	2289	2293	rBV	67510	77567	4.78%	0.619%
47	15.621	2296	2301	2304	rBV	322139	405467	24.97%	3.235%
48	16.109	2380	2384	2391	rVB3	49995	73535	4.53%	0.587%
49	16.645	2471	2475	2481	rBV3	30750	57770	3.56%	0.461%

Sum of corrected areas: 12532341

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Instrument :
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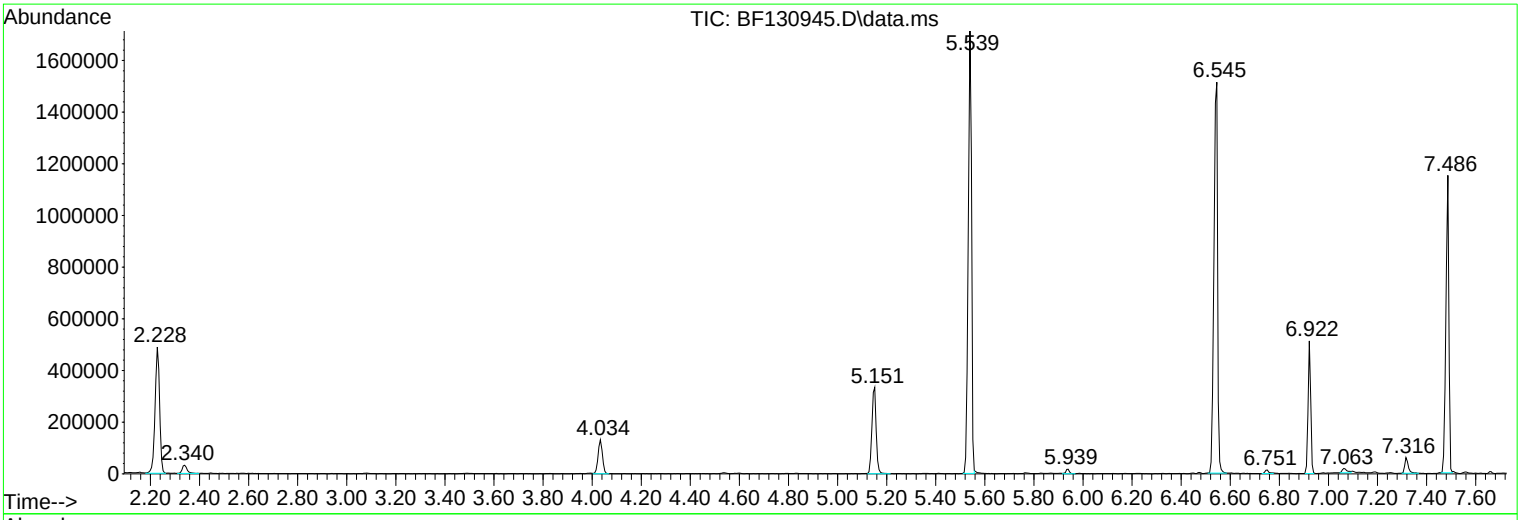
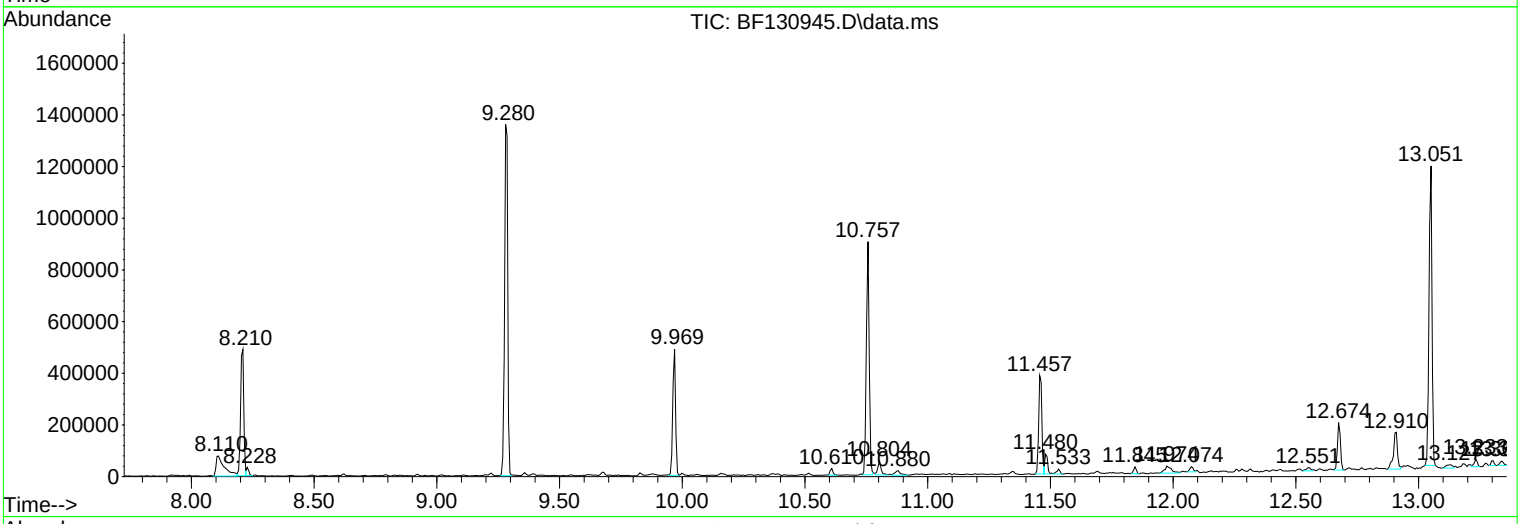
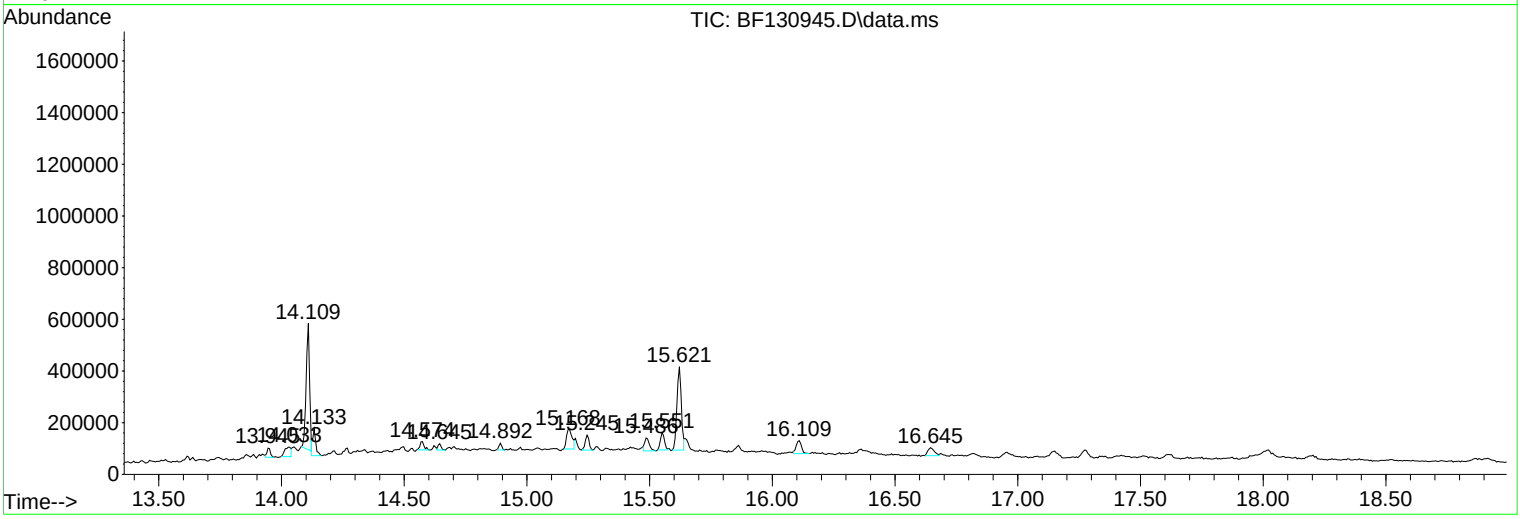
ClientSampleId :
S-4-103122

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

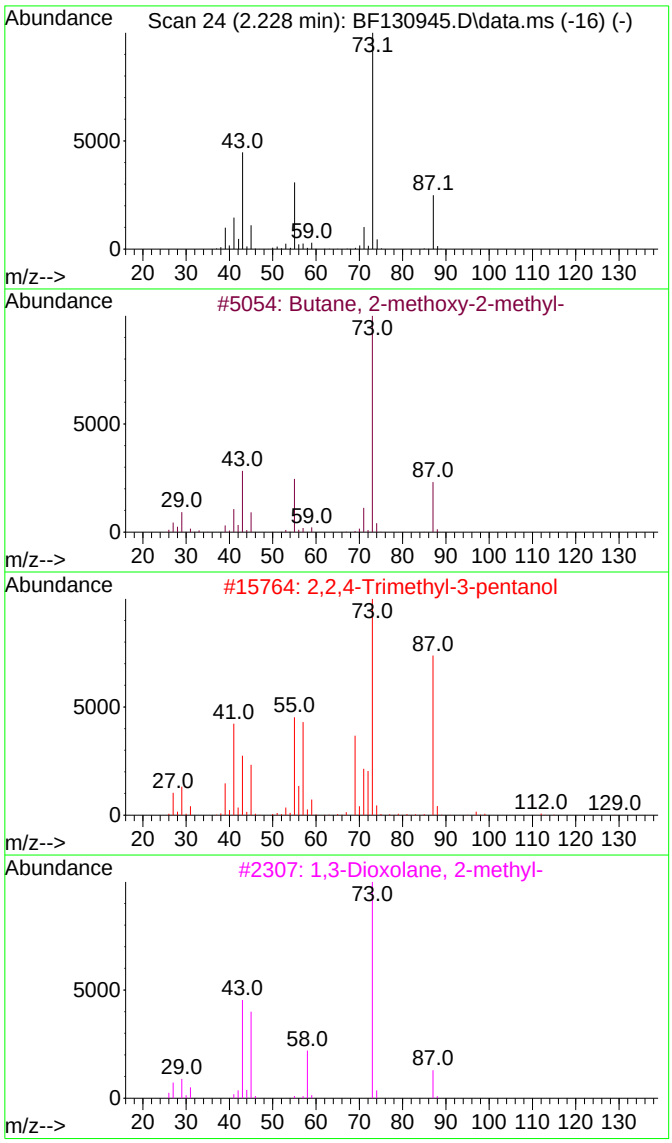
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

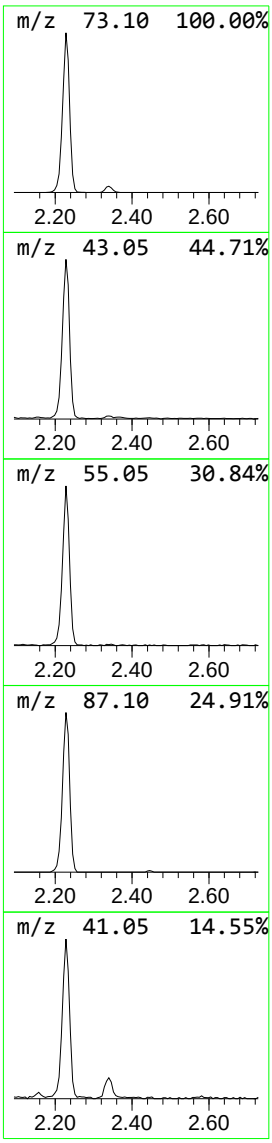
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	32.56 ng	627364	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
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Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-103122

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

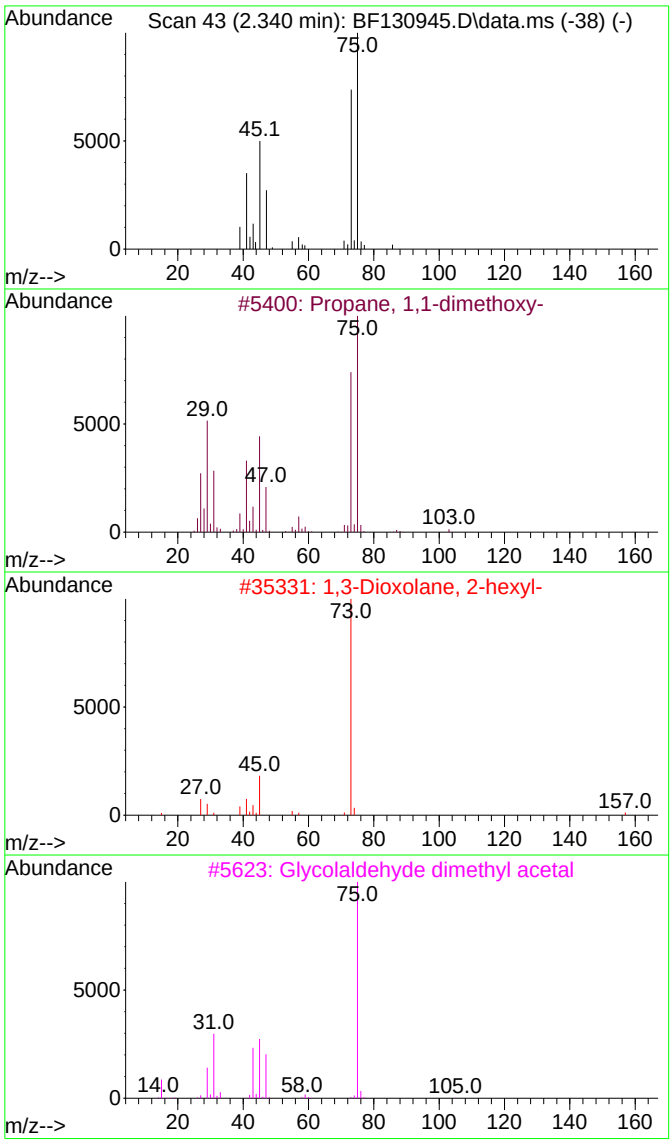
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

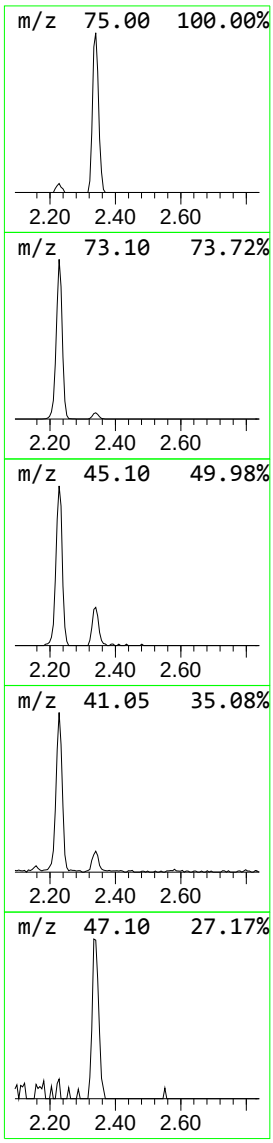
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.340	2.33 ng	44887	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	64
2	1,3-Dioxolane, 2-hexyl-	158	C9H18O2	001708-34-5	9
3	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
4	3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	9
5	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130945.D
Acq On : 02 Nov 2022 23:19
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-103122

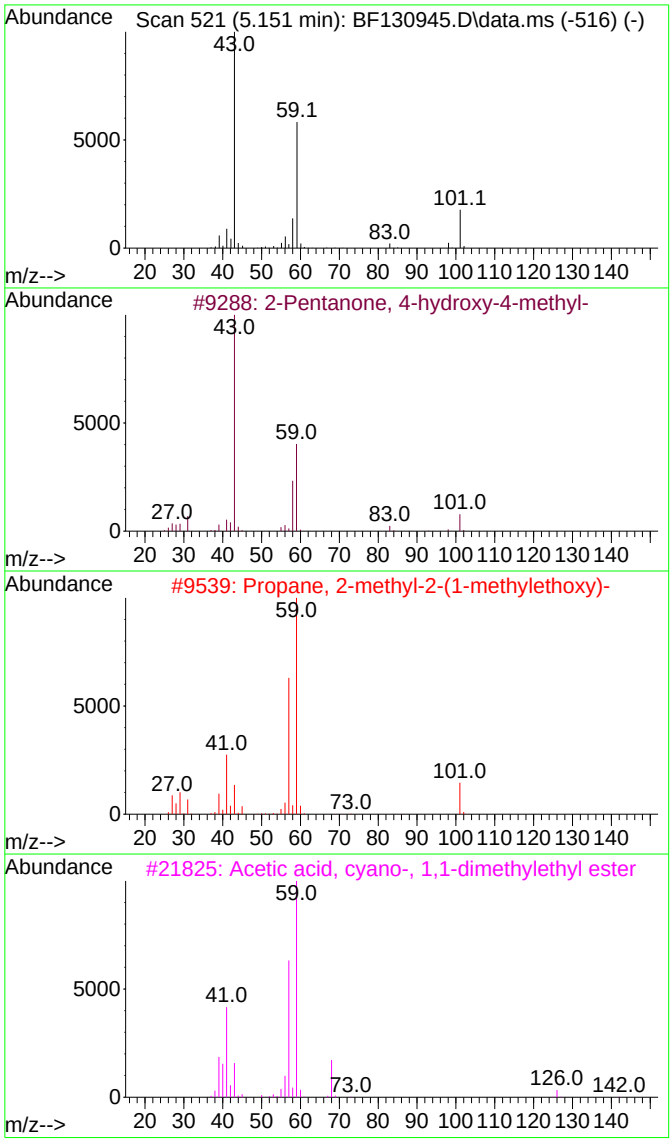
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

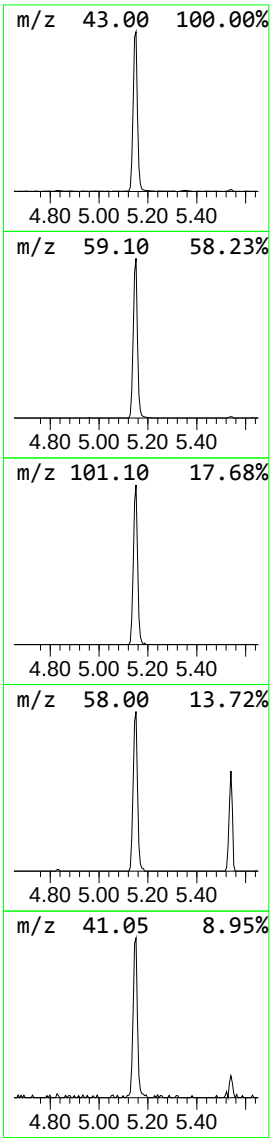
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	20.85 ng	401745	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	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	tert-Butyl carbamate	117	C5H11NO2	004248-19-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-103122

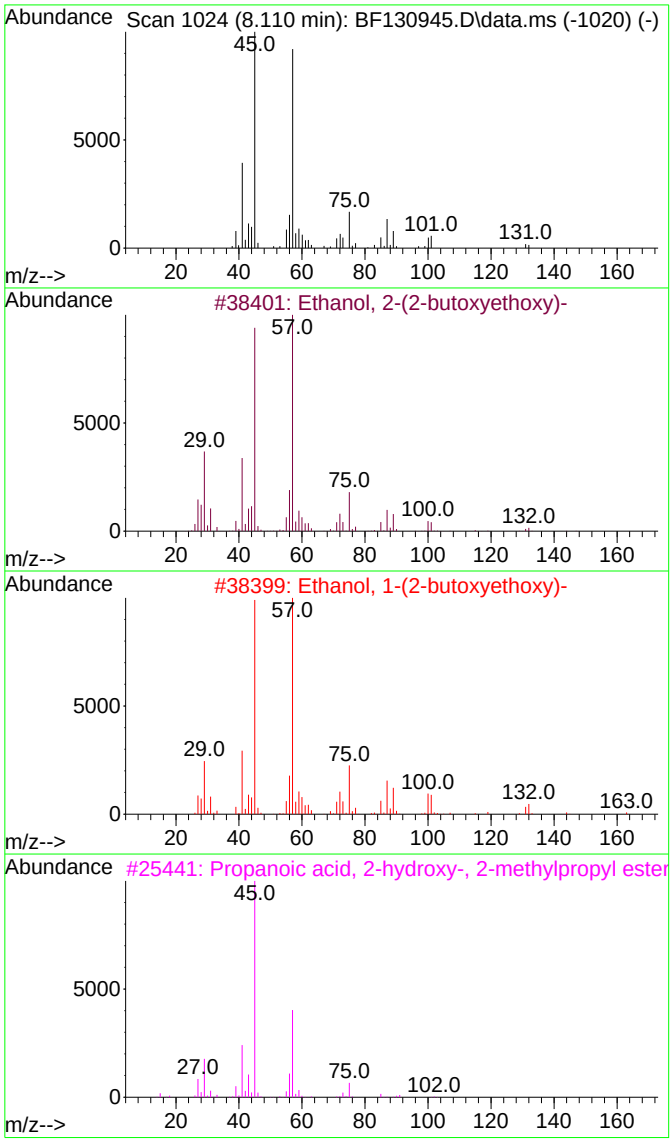
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

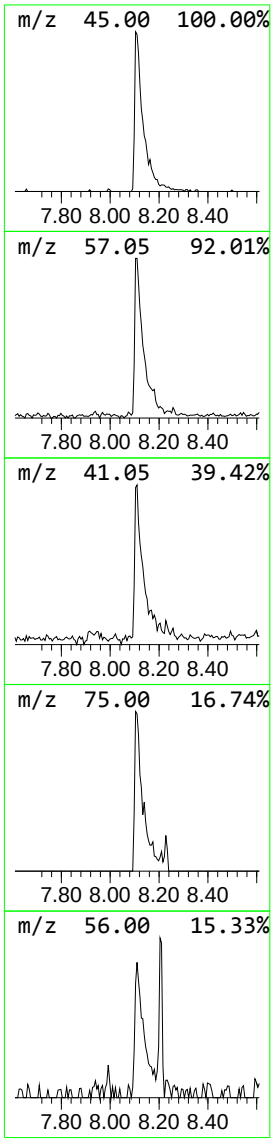
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	8.28 ng	184807	Naphthalene-d8	8.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





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ALS Vial : 15 Sample Multiplier: 1

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

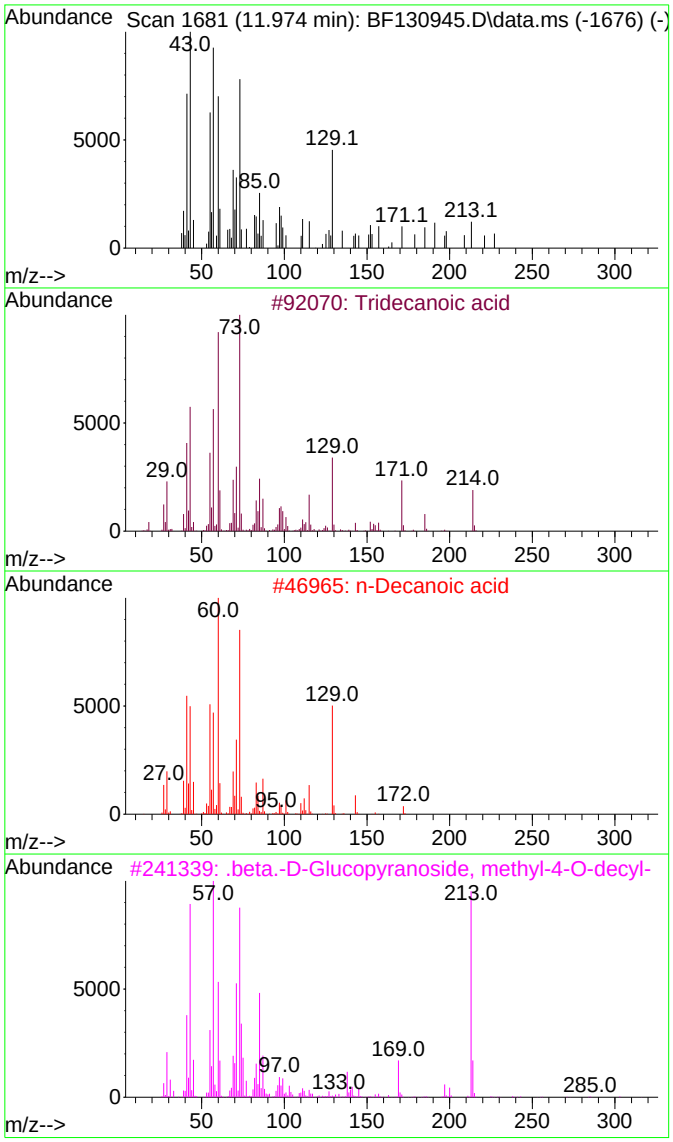
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

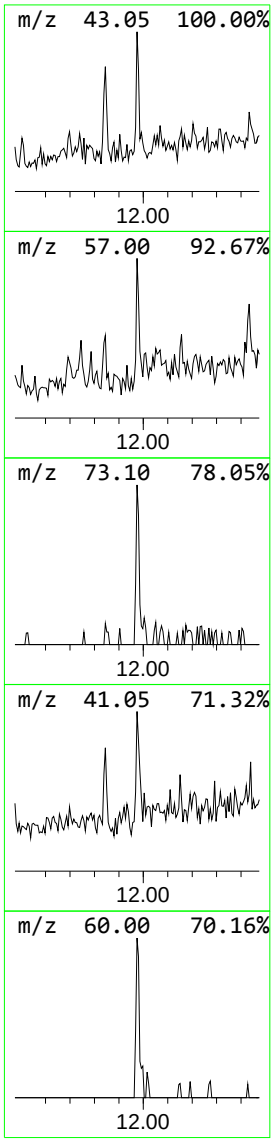
****

Peak Number 6 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.974	3.05 ng	53303	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	50
2	n-Decanoic acid	172	C10H20O2	000334-48-5	46
3	.beta.-D-Glucopyranoside, methyl...	334	C17H34O6	1000157-24-8	38
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35
5	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	35





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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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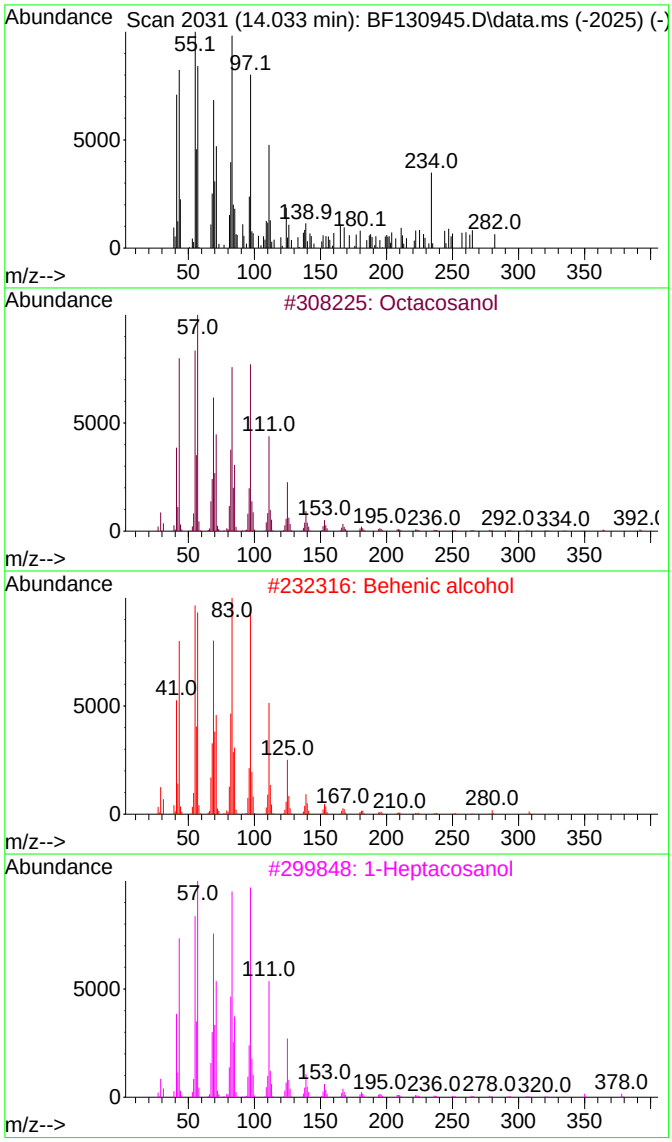
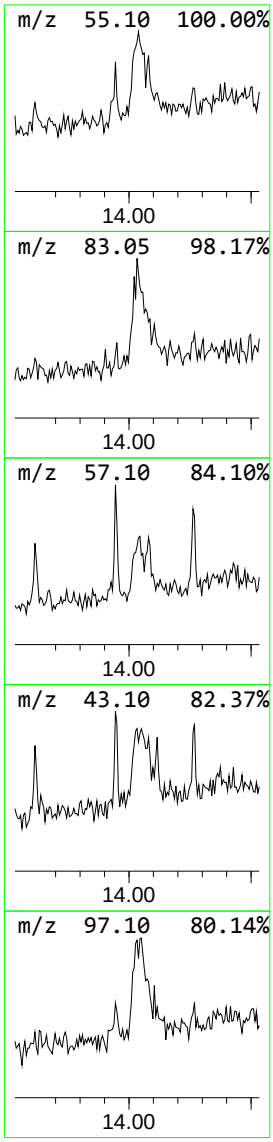
Peak Number 7 Octacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	2.81 ng	67124	Chrysene-d12	14.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	90
2	Behenic alcohol	326	C22H46O	000661-19-8	86
3	1-Heptacosanol	396	C27H56O	002004-39-9	83
4	1-Pentadecanethiol	244	C15H32S	025276-70-4	83
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	83





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Data File : BF130945.D
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Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-103122

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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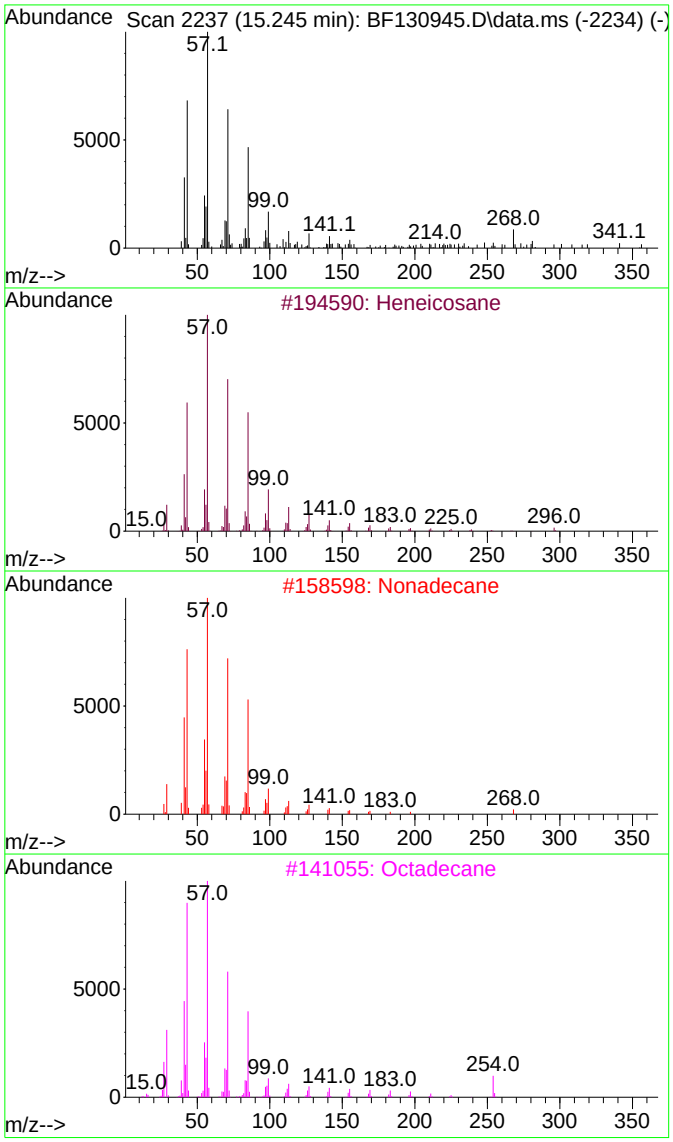
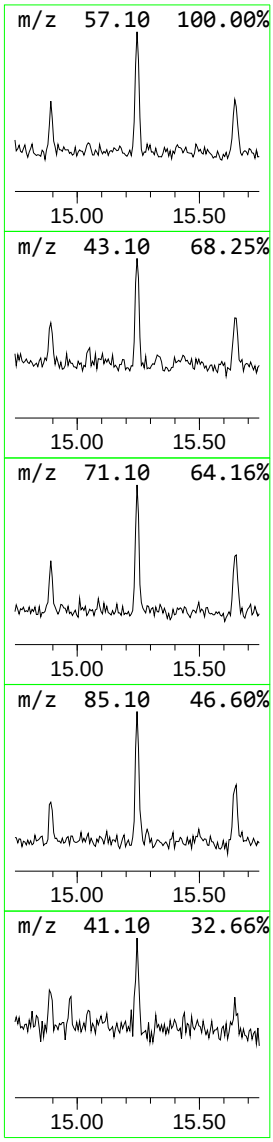
Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	3.05 ng	61733	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Nonadecane	268	C19H40	000629-92-5	93
3	Octadecane	254	C18H38	000593-45-3	90
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130945.D
Acq On : 02 Nov 2022 23:19
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-103122

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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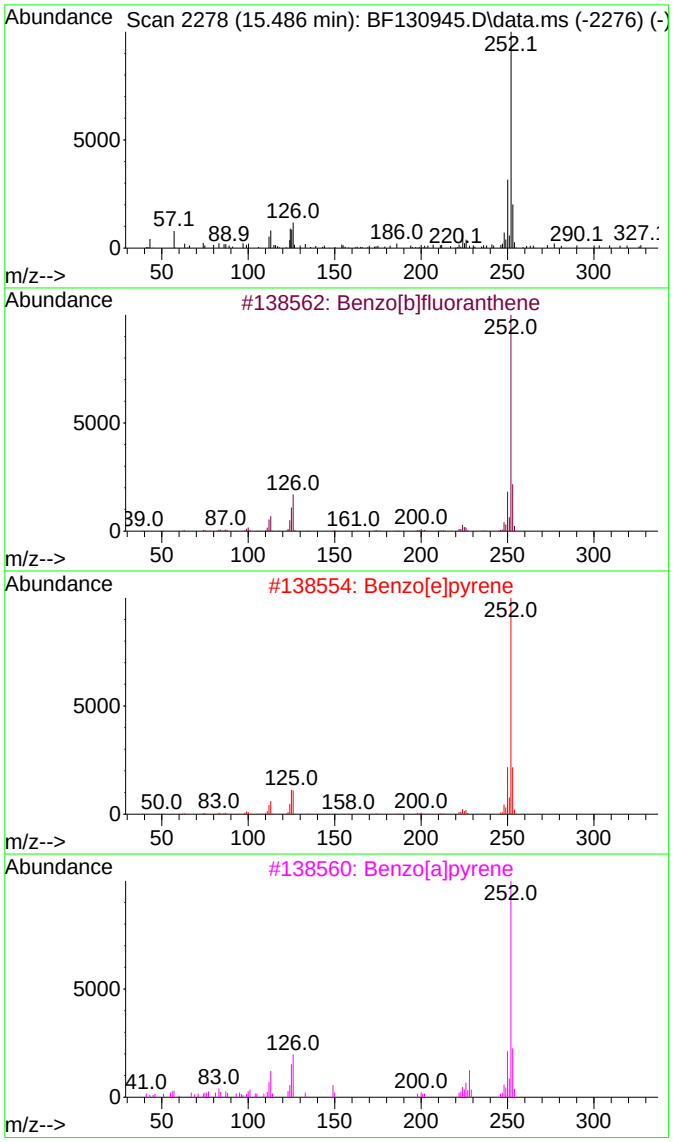
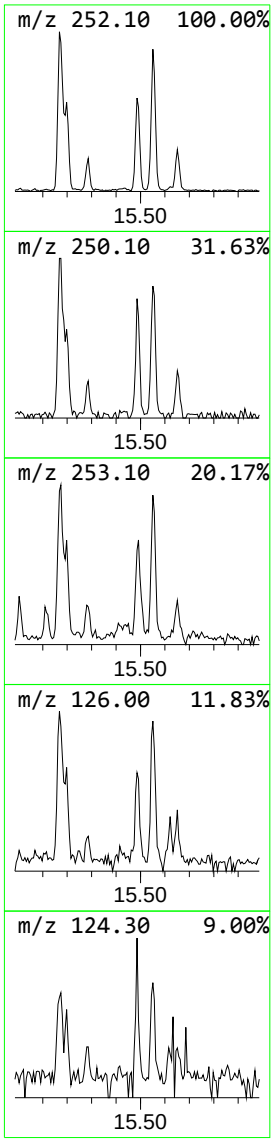
Peak Number 9 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.486	3.21 ng	65080	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
2	Benzo[e]pyrene	252	C20H12	000192-97-2	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	89
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
5	Perylene	252	C20H12	000198-55-0	89





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Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-103122

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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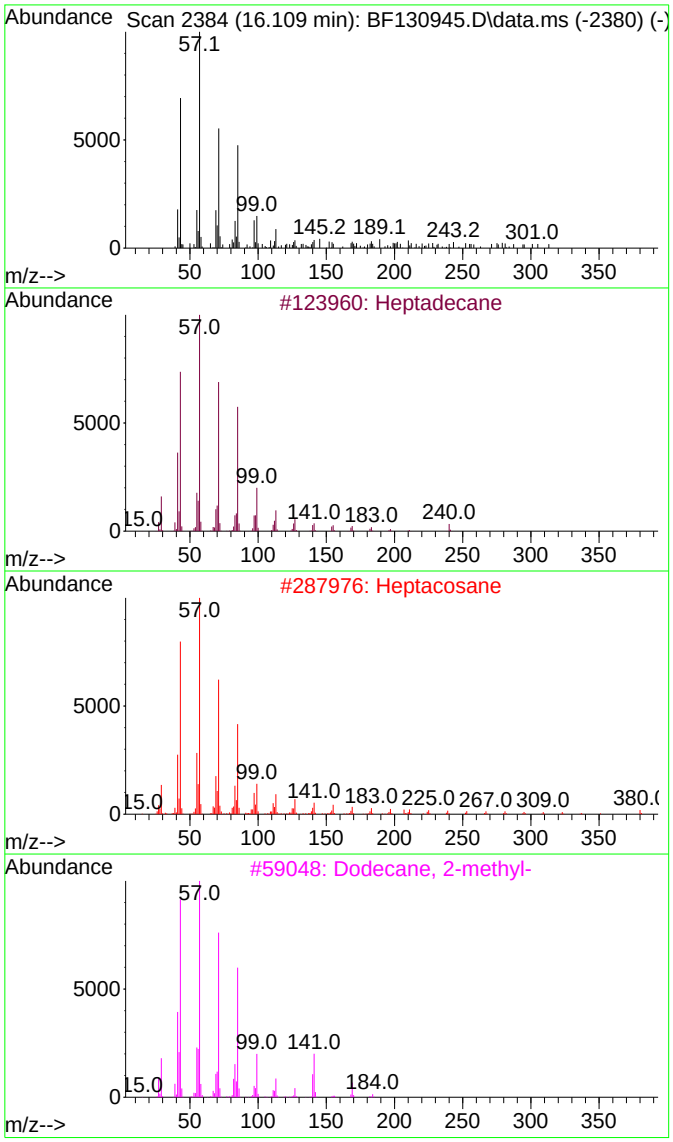
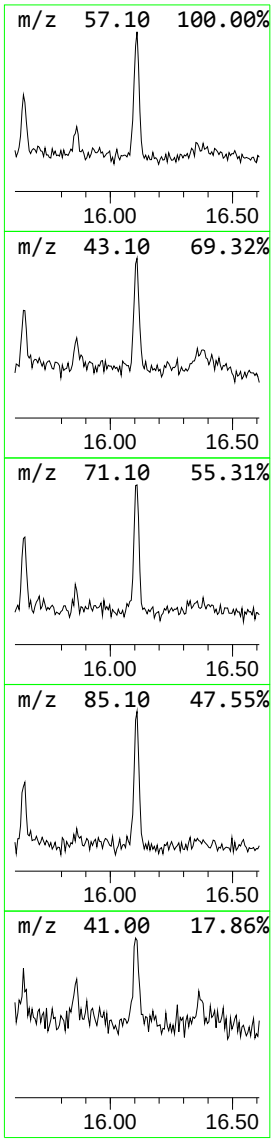
Peak Number 10 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.109	3.63 ng	73535	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	89
2	Heptacosane	380	C27H56	000593-49-7	80
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	76
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72





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Acq On : 02 Nov 2022 23:19
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-103122

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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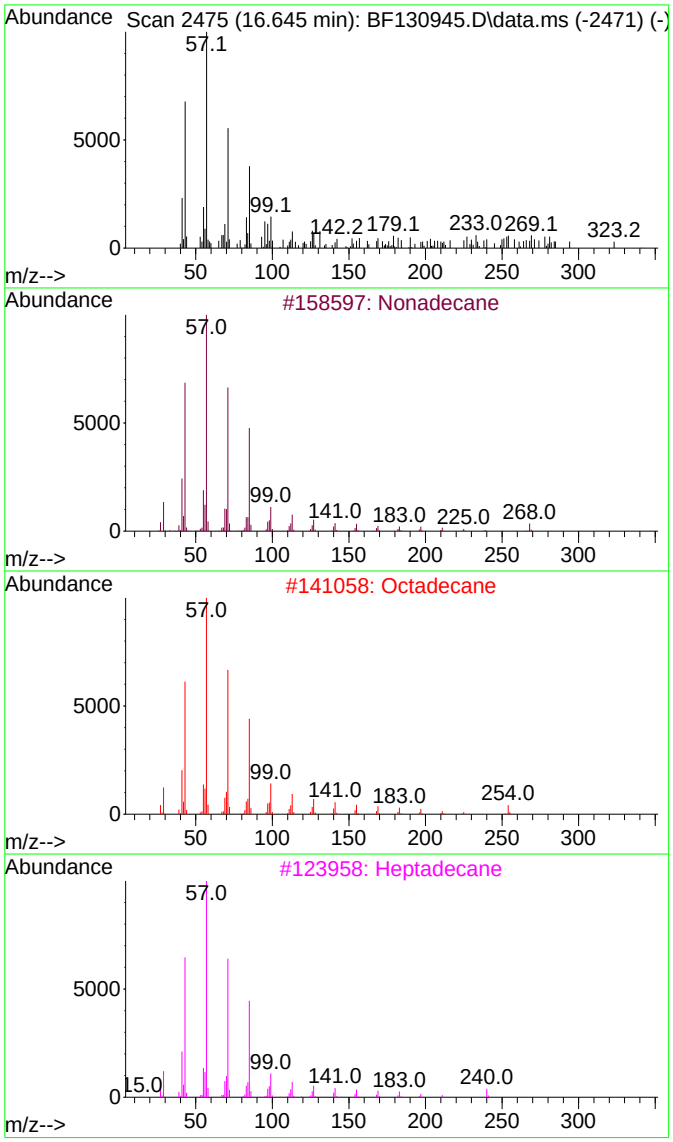
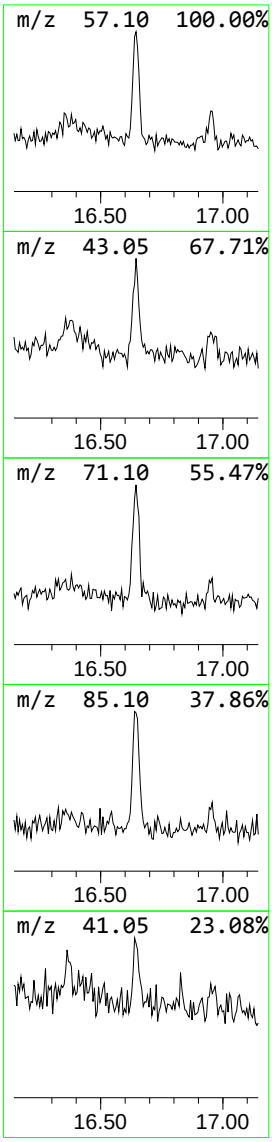
Peak Number 11 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.645	2.85 ng	57770	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Octadecane	254	C18H38	000593-45-3	83
3	Heptadecane	240	C17H36	000629-78-7	78
4	Pentadecane	212	C15H32	000629-62-9	78
5	Eicosane	282	C20H42	000112-95-8	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130945.D
Acq On : 02 Nov 2022 23:19
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-103122

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...	2.228	32.6	ng	627364	1	6.922	385400	20.0
Propane, 1,1-di...	2.340	2.3	ng	44887	1	6.922	385400	20.0
2-Pentanone, 4-...	5.151	20.9	ng	401745	1	6.922	385400	20.0
Ethanol, 2-(2-b...	8.110	8.3	ng	184807	2	8.210	446283	20.0
Tridecanoic acid	11.974	3.0	ng	53303	4	11.457	349068	20.0
Octacosanol	14.033	2.8	ng	67124	5	14.110	477521	20.0
Heneicosane	15.245	3.0	ng	61733	6	15.621	405467	20.0
Benzo[e]pyrene	15.486	3.2	ng	65080	6	15.621	405467	20.0
Heptadecane	16.109	3.6	ng	73535	6	15.621	405467	20.0
Nonadecane	16.645	2.9	ng	57770	6	15.621	405467	20.0