LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130960.D
Acq On : 03 Nov 2022 13:27
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 8 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: BF130960.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	18	26	31	rBV	468449	610211	35.39%	4.397%
2	2.346	38	44	53	rBV	29620	38405	2.23%	0.277%
3	4.040	327	332	337	rVB	125846	156736	9.09%	1.129%
4	5.151	516	521	533	rVB	359603	423635	24.57%	3.053%
5	5.545	582	588	591	rBV	1762247	1724377	100.00%	12.426%
6	6.545	752	758	761	rBV	1708443	1716491	99.54%	12.369%
7	6.745	789	792	802	rBV3	15409	21278	1.23%	0.153%
8	6.922	818	822	825	rBV	537136	406013	23.55%	2.926%
9	7.069	843	847	864	rBV7	16538	45541	2.64%	0.328%
10	7.316	885	889	899	rBV	62390	69854	4.05%	0.503%
11	7.487	913	918	921	rBV	1207620	1083190	62.82%	7.806%
12	8.110	1020	1024	1037	rBV	83474	208489	12.09%	1.502%
13	8.204	1037	1040	1043	rVV	526718	507139	29.41%	3.654%
14	8.228	1043	1044	1047	rVB	34746	20786	1.21%	0.150%
15	9.286	1218	1224	1227	rBV	1592125	1450411	84.11%	10.452%
16	9.969	1334	1340	1343	rBV	578734	486686	28.22%	3.507%
17	10.157	1369	1372	1379	rVB4	13538	20680	1.20%	0.149%
18	10.610	1446	1449	1455	rVB	32745	28825	1.67%	0.208%
19	10.757	1470	1474	1479	rBV	1097792	921066	53.41%	6.637%
20	10.804	1479	1482	1489	rVB	49017	51956	3.01%	0.374%
21	10.875	1489	1494	1497	rBV	21600	23265	1.35%	0.168%
22	11.345	1571	1574	1581	rVB4	14004	18098	1.05%	0.130%
23	11.457	1590	1593	1596	rBV	463287	426401	24.73%	3.073%
24	11.480	1596	1597	1600	rVV	94199	69386	4.02%	0.500%
25	11.533	1602	1606	1609	rVB	23553	25581	1.48%	0.184%
26	11.686	1628	1632	1637	rBV2	17744	24607	1.43%	0.177%
27	11.845	1655	1659	1662	rBV	34986	31027	1.80%	0.224%
28	11.974	1677	1681	1687	rBV3	33043	57597	3.34%	0.415%
29	12.074	1694	1698	1700	rBV2	23319	22427	1.30%	0.162%
30	12.257	1725	1729	1732	rBV2	20828	23020	1.33%	0.166%
31	12.551	1775	1779	1782	rBV5	12340	20403	1.18%	0.147%
32	12.674	1797	1800	1804	rBV	185184	154015	8.93%	1.110%
33	12.910	1834	1840	1843	rBV	144436	169815	9.85%	1.224%
34	13.051	1857	1864	1867	rBV	1053109	987169	57.25%	7.114%
35	13.116	1872	1875	1881	rBV7	13130	24209	1.40%	0.174%
36	13.186	1884	1887	1889	rBV3	16846	20384	1.18%	0.147%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130960.D
Acq On : 03 Nov 2022 13:27
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 8 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	13.233	1893	1895	1898	rVB	26421	25047	1.45%	0.180%
38	13.945	2014	2016	2021	rVB3	28795	28837	1.67%	0.208%
39	14.027	2025	2030	2036	rVV7	39832	117911	6.84%	0.850%
40	14.110	2039	2044	2046	rVV2	438867	488267	28.32%	3.518%
41	14.133	2046	2048	2053	rVB	91423	79946	4.64%	0.576%
42	14.204	2057	2060	2065	rVB2	53957	63766	3.70%	0.460%
43	14.263	2068	2070	2073	rVB3	19562	18350	1.06%	0.132%
44	14.568	2120	2122	2125	rBV2	29623	22754	1.32%	0.164%
45	15.168	2220	2224	2228	rBV	77307	123379	7.15%	0.889%
46	15.245	2233	2237	2240	rVB	51948	63614	3.69%	0.458%
47	15.486	2275	2278	2283	rVB	54357	73709	4.27%	0.531%
48	15.551	2285	2289	2295	rBV	71484	94500	5.48%	0.681%
49	15.621	2296	2301	2305	rBV	316683	422565	24.51%	3.045%
50	16.104	2380	2383	2388	rVB	49468	69684	4.04%	0.502%
51	16.639	2470	2474	2481	rBV2	27019	45057	2.61%	0.325%
52	17.615	2635	2640	2647	rVB2	24681	50671	2.94%	0.365%

Sum of corrected areas: 13877230

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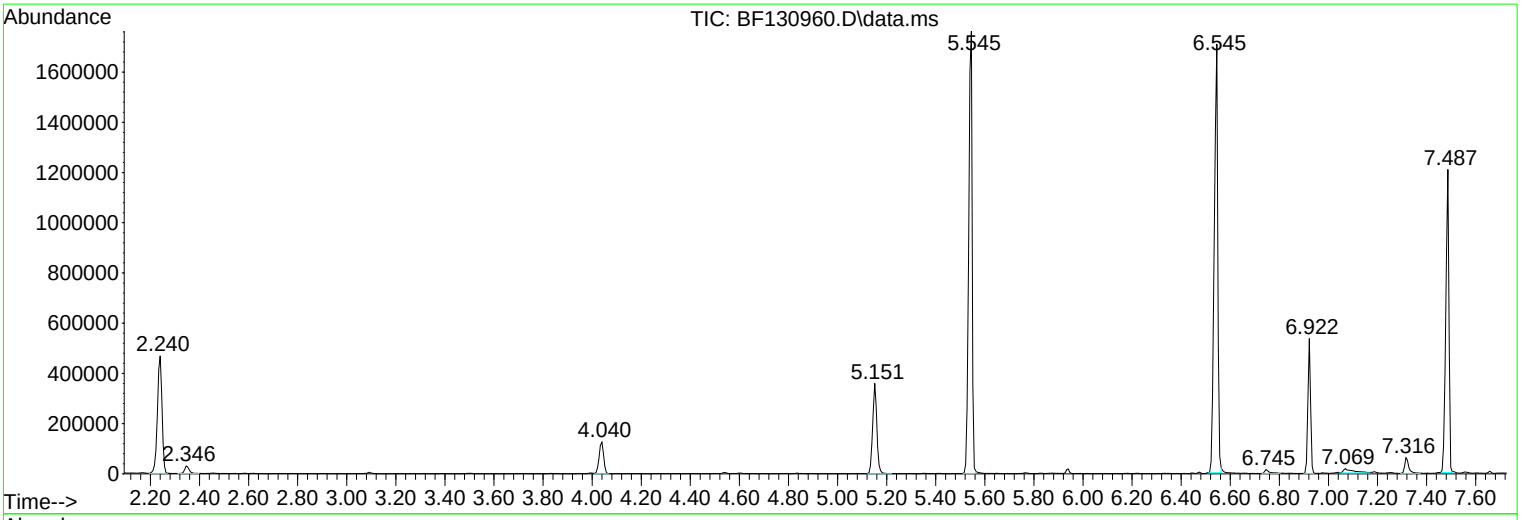
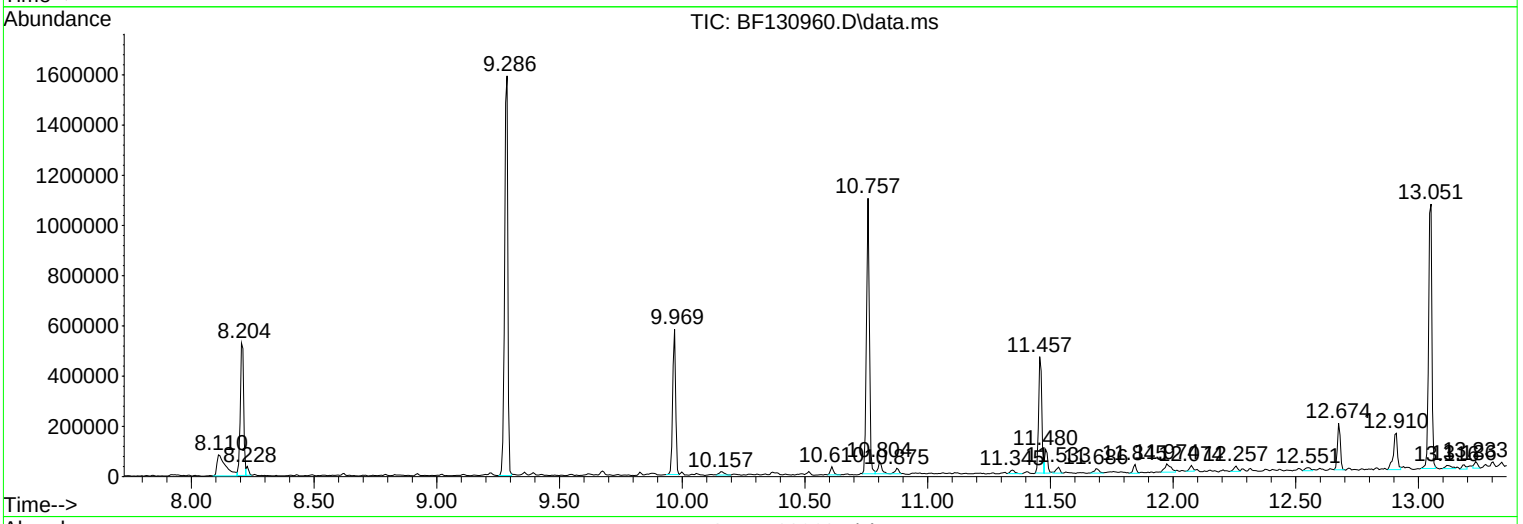
ALS Vial : 8 Sample Multiplier: 1

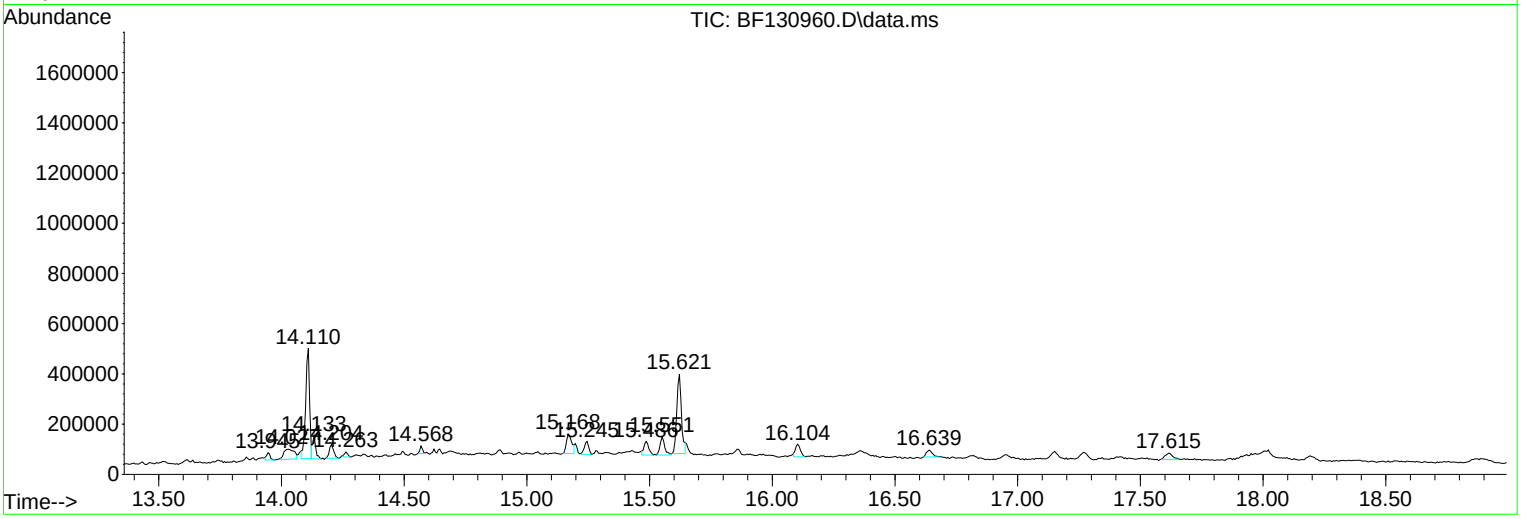
Instrument :
BNA_F
ClientSampleId :
S-4-103122

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130960.D
Acq On : 03 Nov 2022 13:27
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 8 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

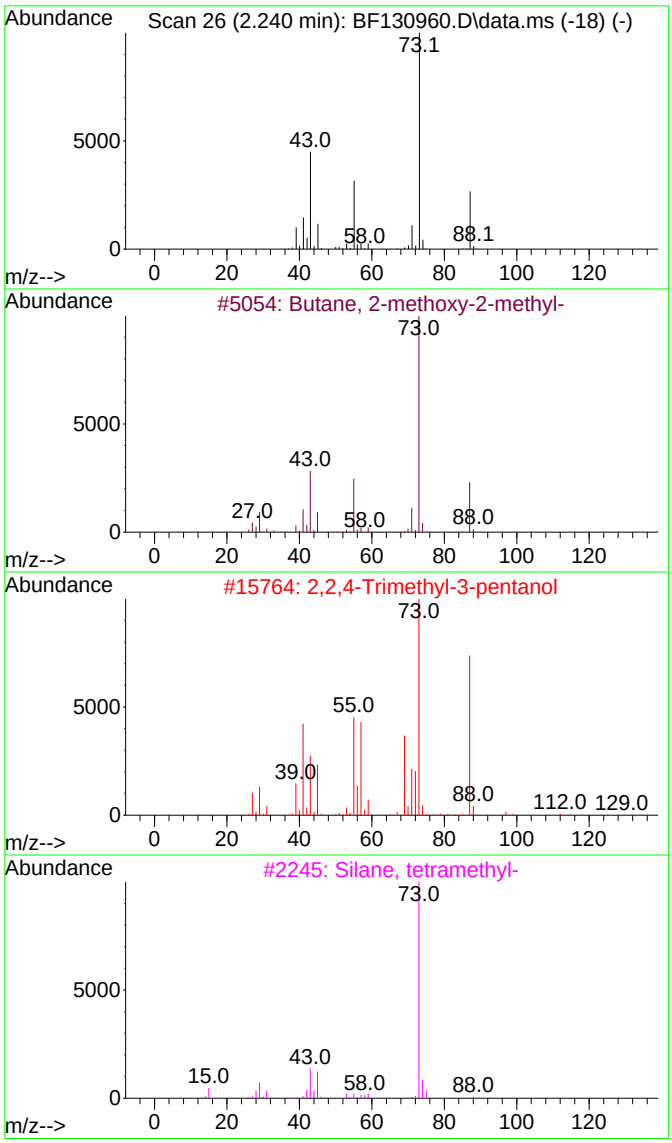
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

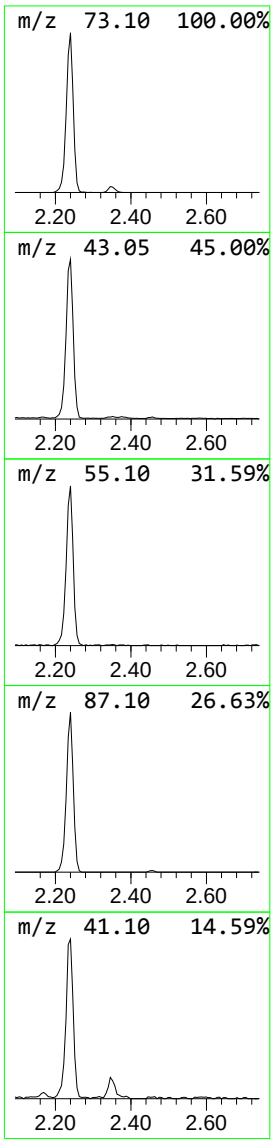
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	30.06 ng	610211	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	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130960.D
Acq On : 03 Nov 2022 13:27
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-103122

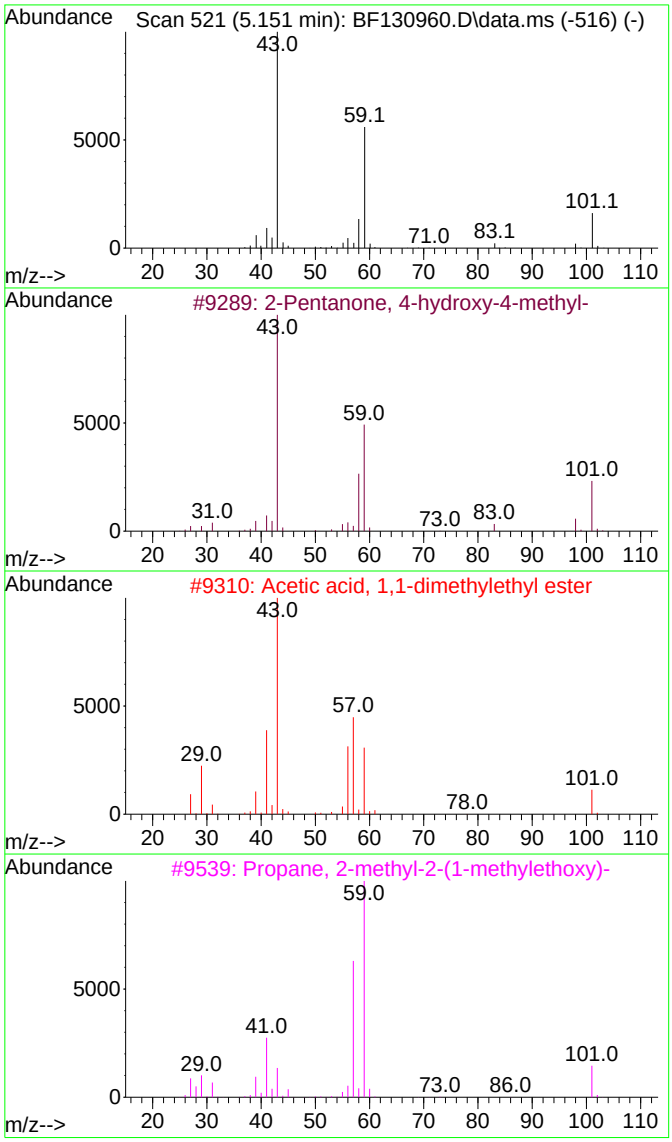
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

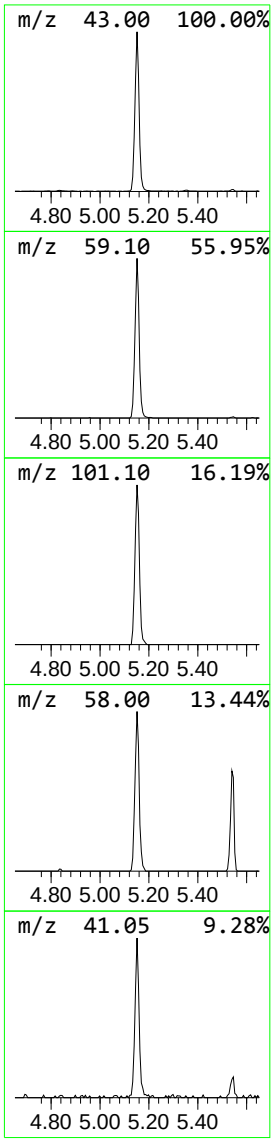
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	20.87 ng	423635	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	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130960.D
Acq On : 03 Nov 2022 13:27
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 8 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

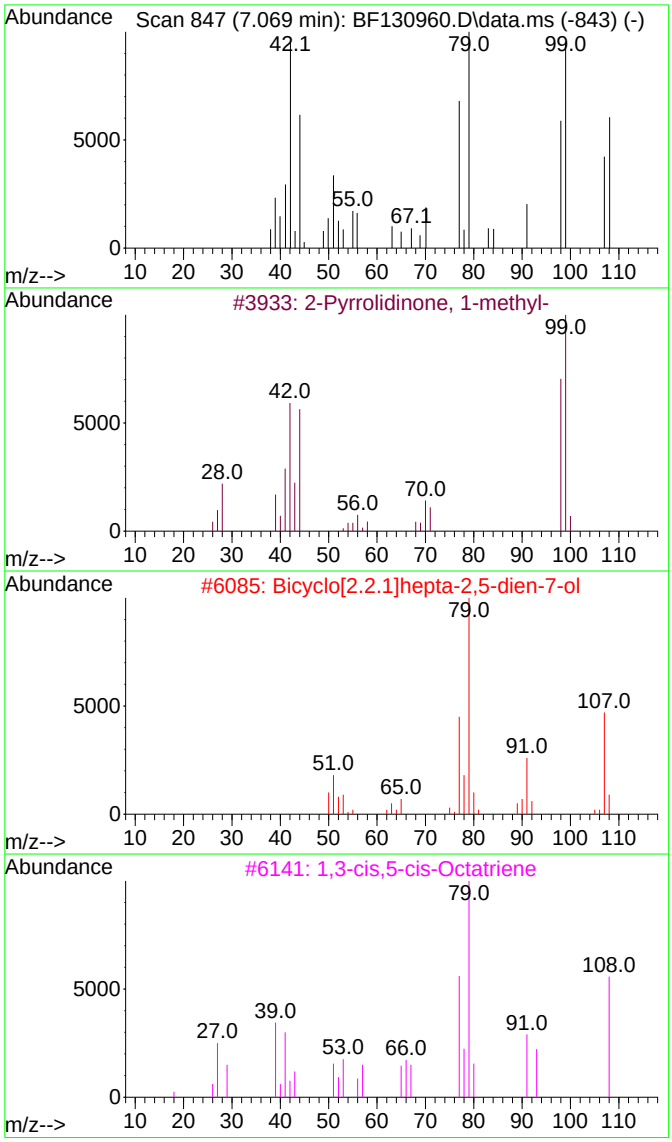
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

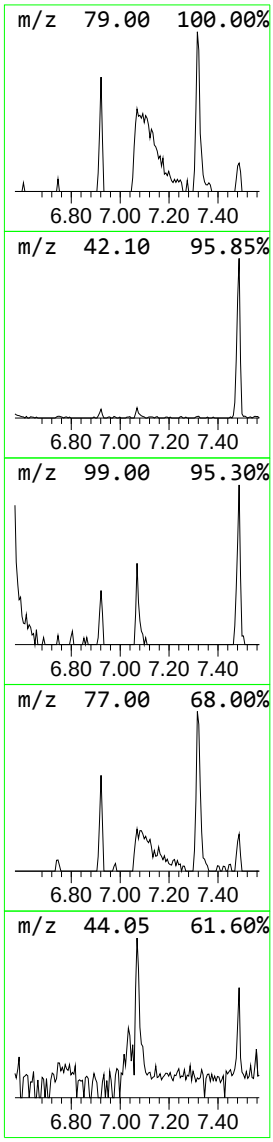
****

Peak Number 4 unknown7.069 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	2.24 ng	45541	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	43
2	Bicyclo[2.2.1]hepta-2,5-dien-7-ol	108	C7H8O	000822-80-0	35
3	1,3-cis,5-cis-Octatriene	108	C8H12	040087-62-5	22
4	Ethanone, 1-phenyl-2-(1-piperidi...	203	C13H17NO	000779-52-2	12
5	5-Methyl-1,2,4-oxadiazol-3-amine	99	C3H5N3O	040483-47-4	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
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Sample : N5395-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-4-103122

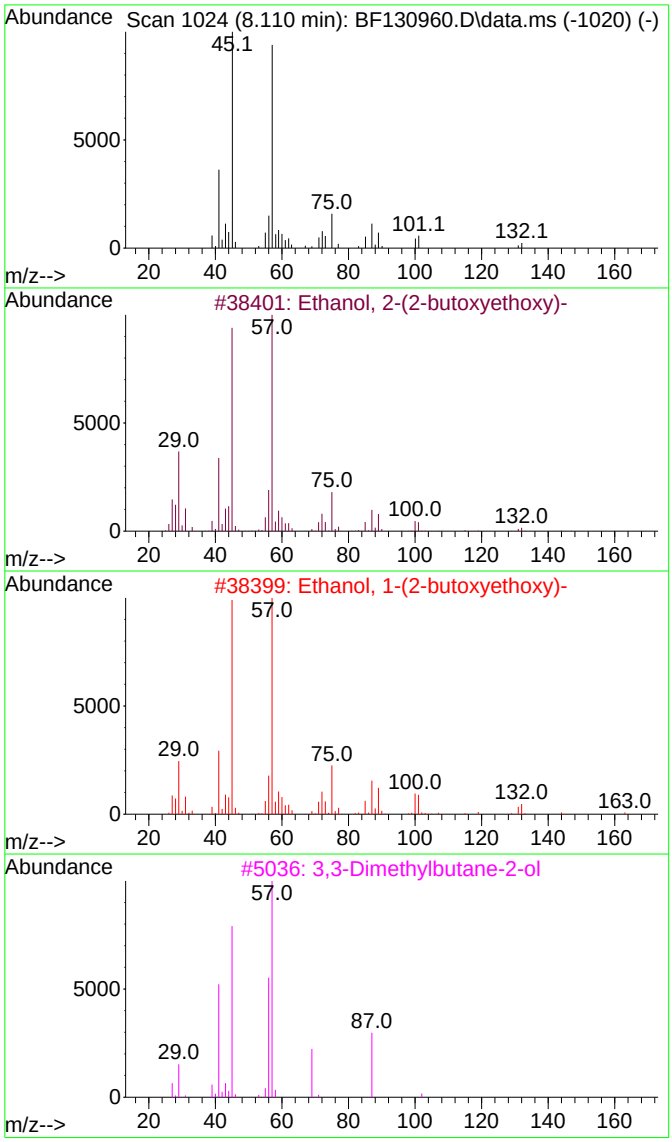
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

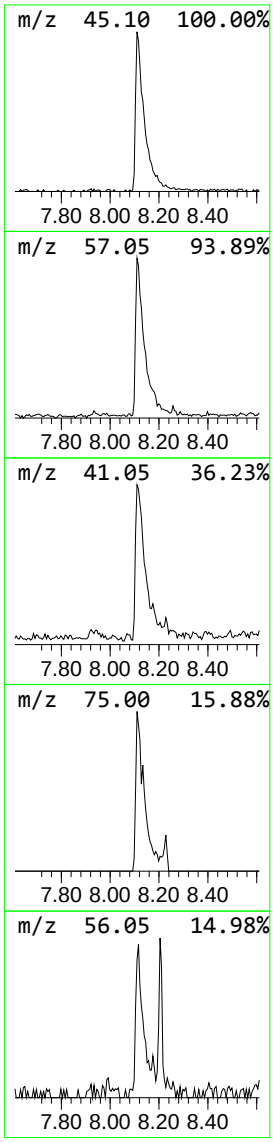
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	8.22 ng	208489	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	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50





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Operator : CG\JU
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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

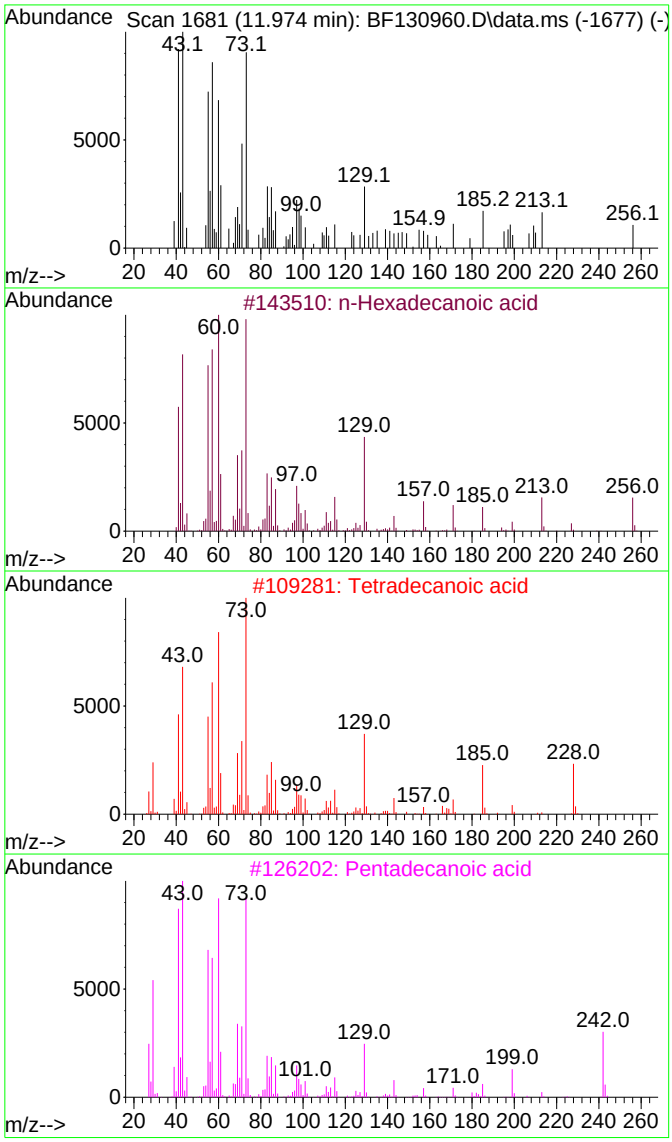
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

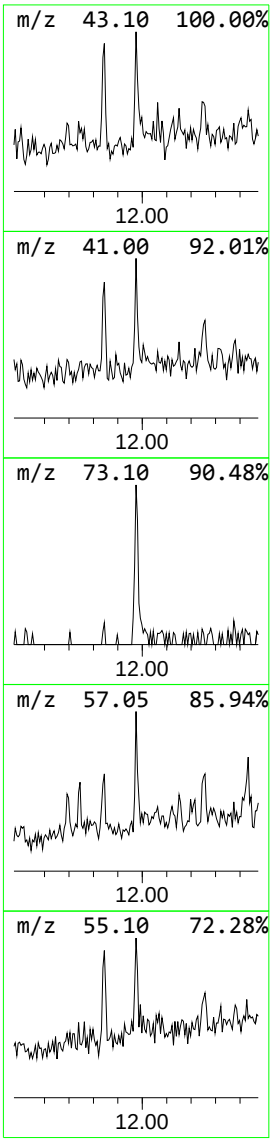
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.975	2.70 ng	57597	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
4	Dodecanoic acid	200	C12H24O2	000143-07-7	38
5	Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	27





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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

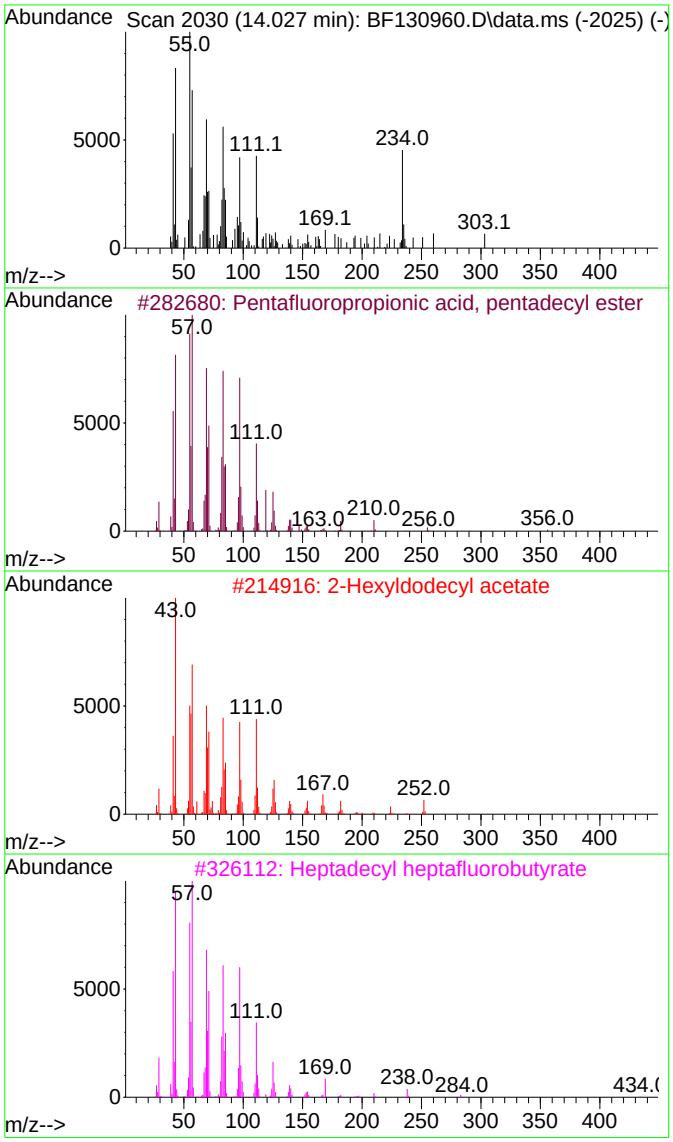
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

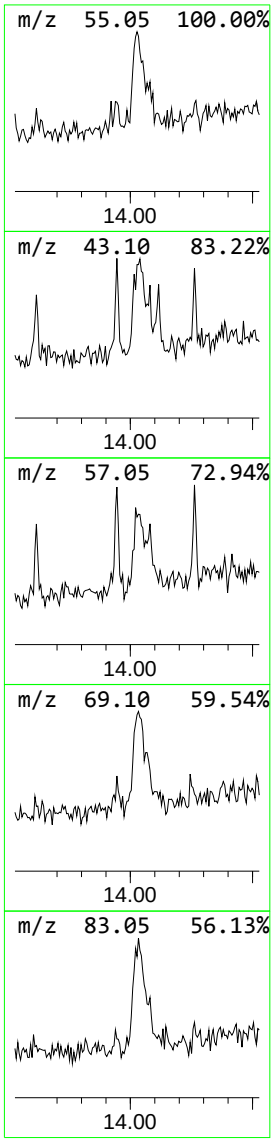
****

Peak Number 7 unknown14.027 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.027	4.83 ng	117911	Chrysene-d12	14.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	49
2	2-Hexyldodecyl acetate	312	C20H40O2	1000368-55-9	46
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	46
4	Cyclopentadecane	210	C15H30	000295-48-7	46
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	46





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Data File : BF130960.D
Acq On : 03 Nov 2022 13:27
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 8 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

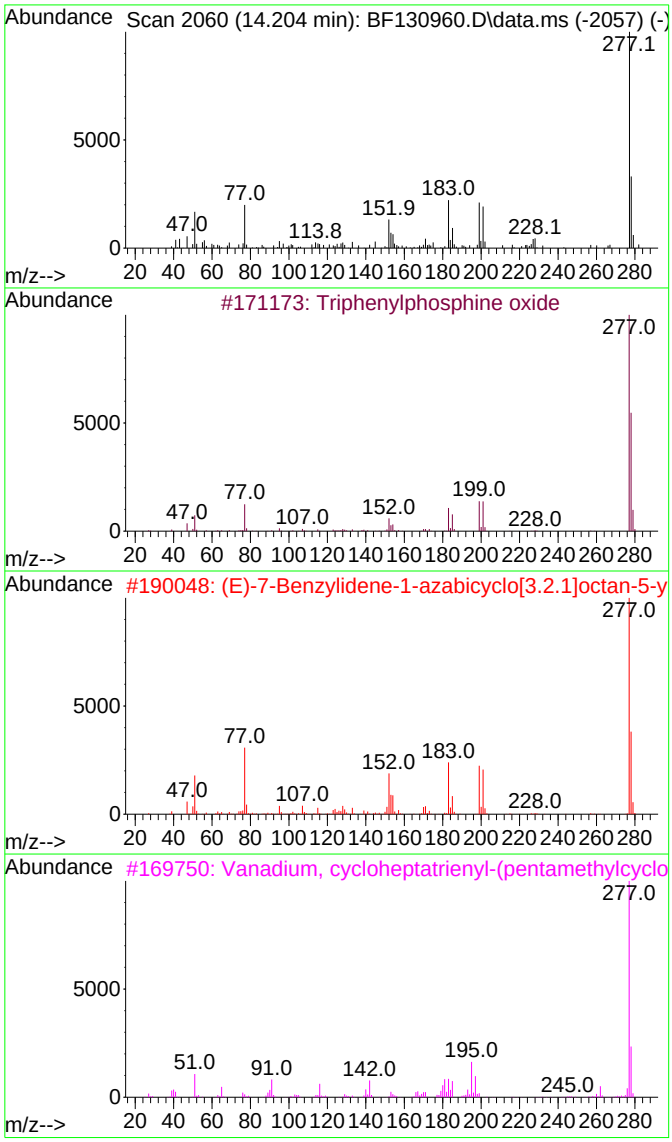
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

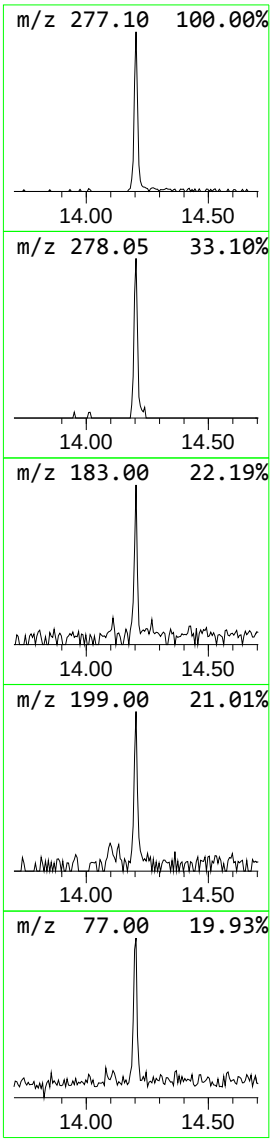
****

Peak Number 8 Triphenylphosphine oxide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.204	2.61 ng	63766	Chrysene-d12	14.110

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	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130960.D
Acq On : 03 Nov 2022 13:27
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 8 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

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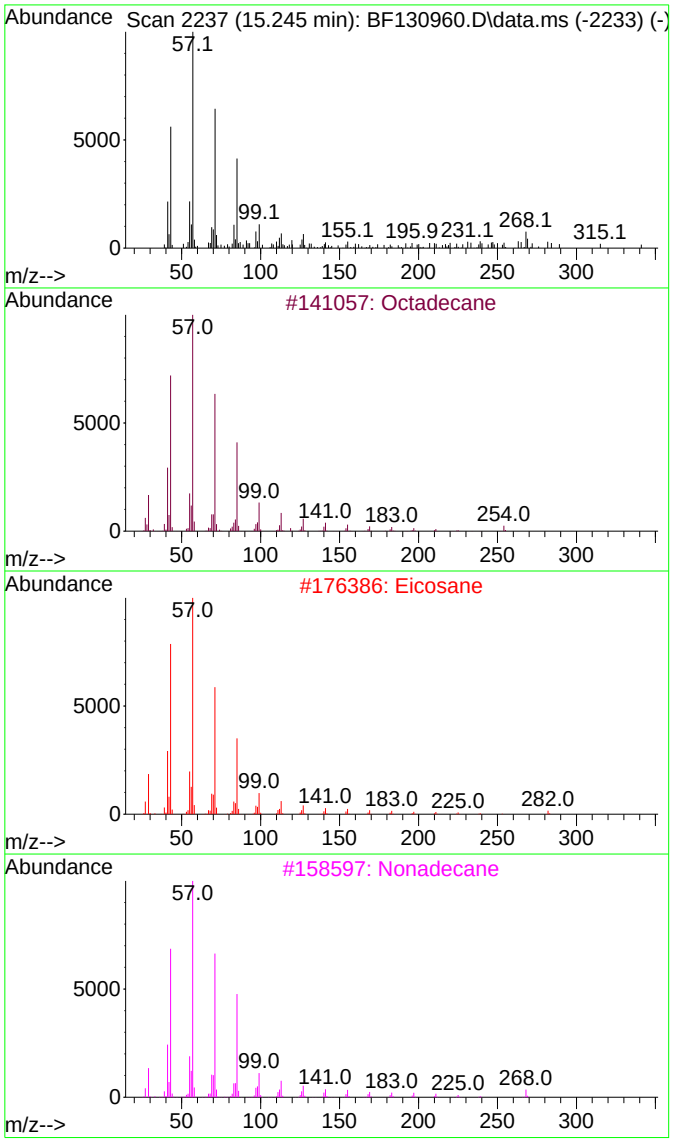
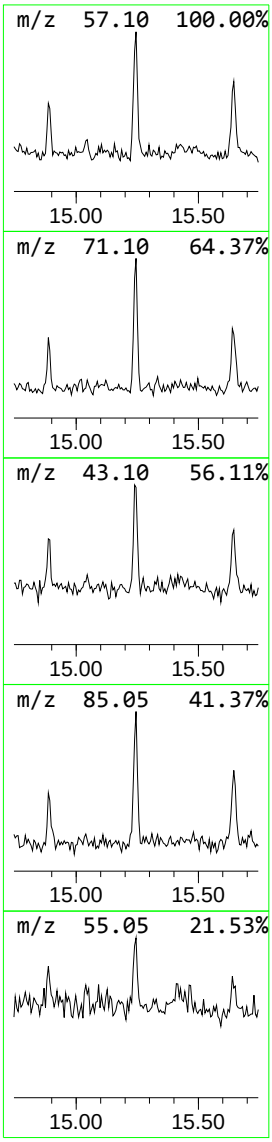
Peak Number 9 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	3.01 ng	63614	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Eicosane	282	C20H42	000112-95-8	91
3	Nonadecane	268	C19H40	000629-92-5	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Heptacosane	380	C27H56	000593-49-7	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130960.D
Acq On : 03 Nov 2022 13:27
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 8 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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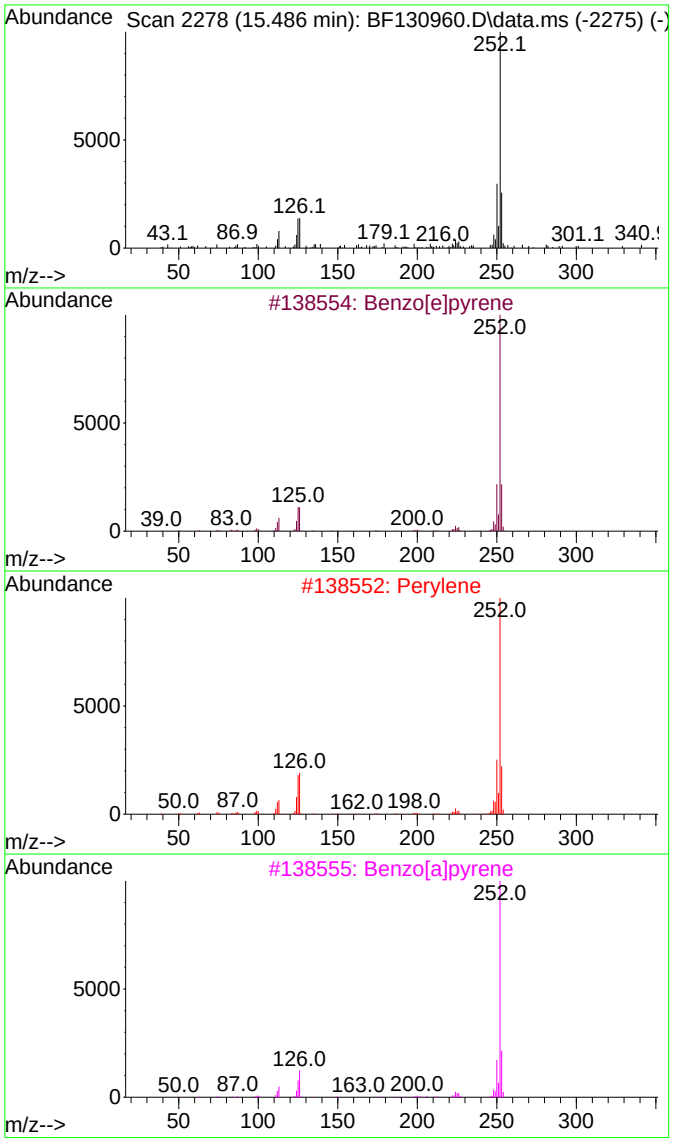
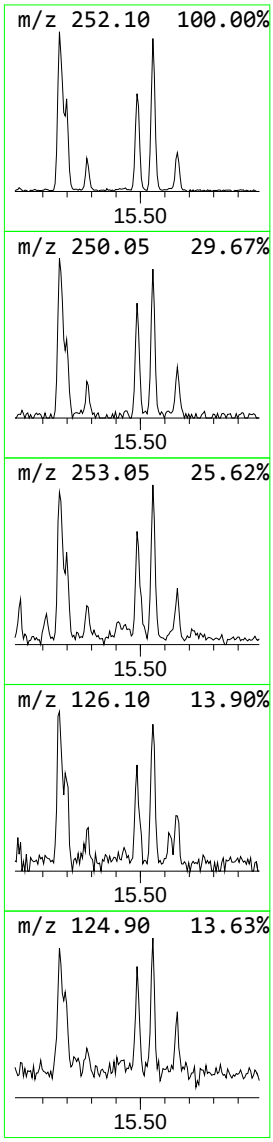
Peak Number 10 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.486	3.49 ng	73709	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Perylene	252	C20H12	000198-55-0	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130960.D
Acq On : 03 Nov 2022 13:27
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 8 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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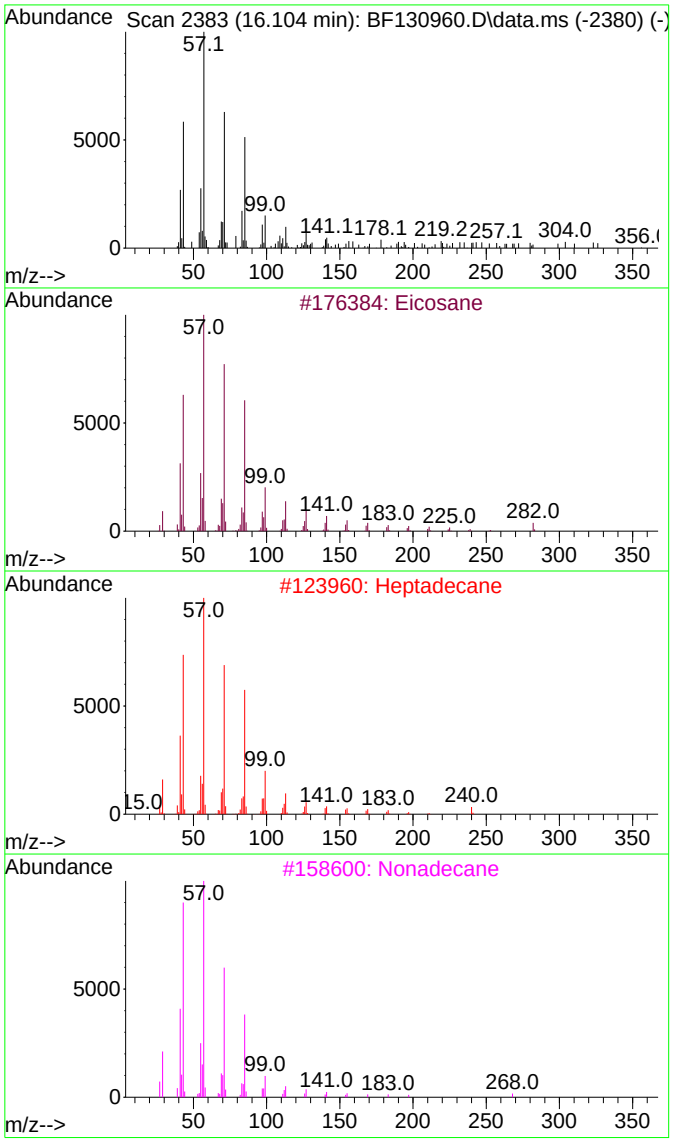
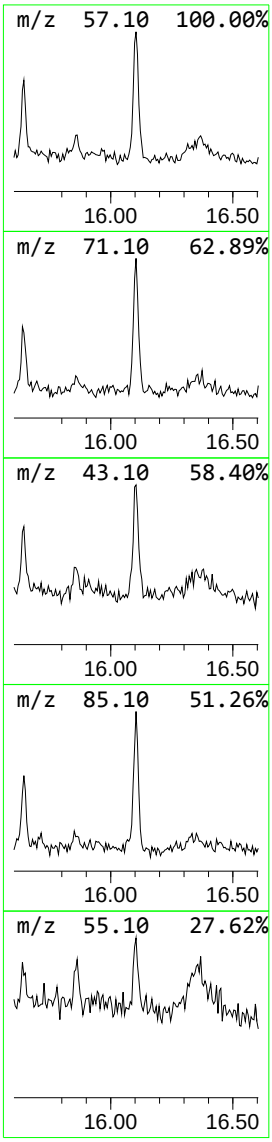
Peak Number 11 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	3.30 ng	69684	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Heptadecane	240	C17H36	000629-78-7	87
3	Nonadecane	268	C19H40	000629-92-5	86
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130960.D
Acq On : 03 Nov 2022 13:27
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 8 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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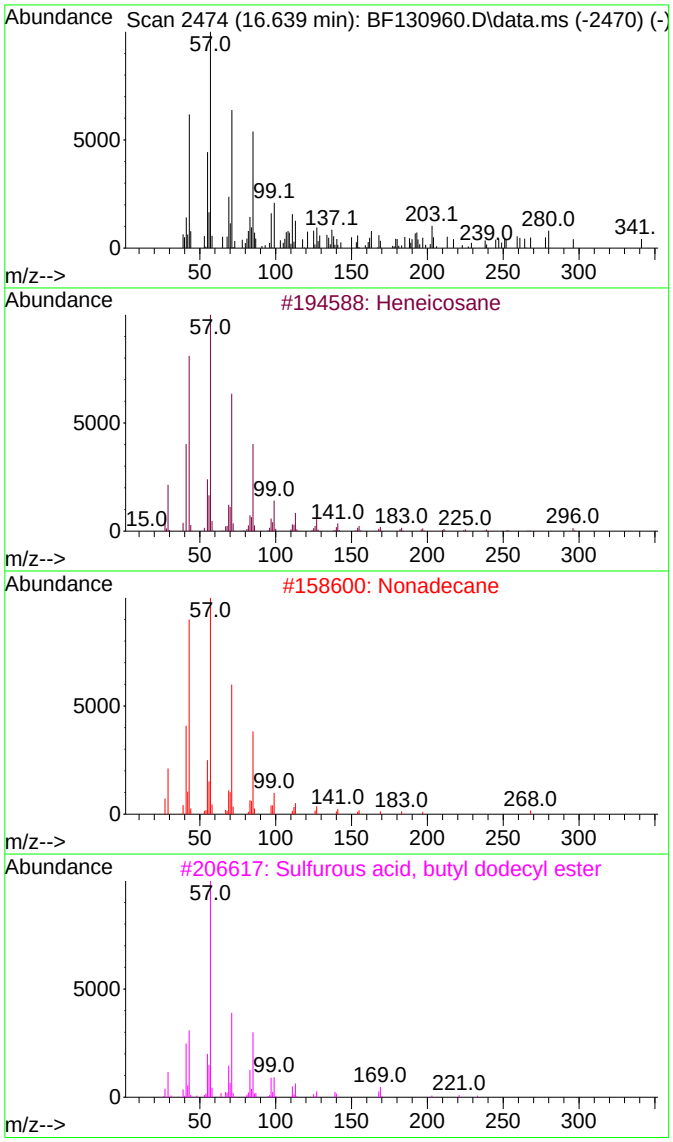
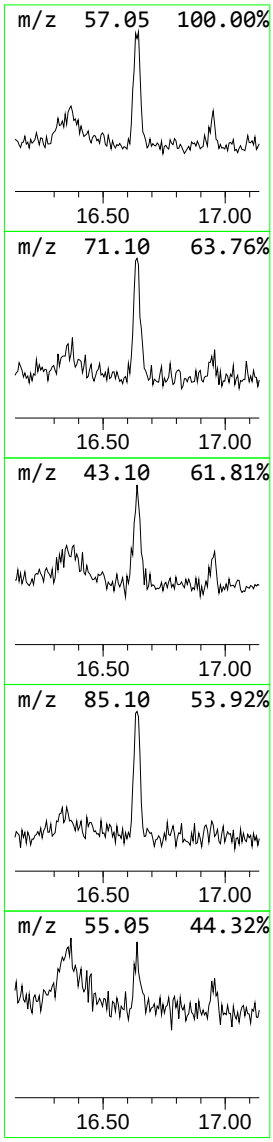
Peak Number 12 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.639	2.13 ng	45057	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	89
2	Nonadecane	268	C19H40	000629-92-5	89
3	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	64
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	64
5	Heptacosane	380	C27H56	000593-49-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130960.D
Acq On : 03 Nov 2022 13:27
Operator : CG\JU
Sample : N5395-05
Misc :
ALS Vial : 8 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...	2.240	30.1	ng	610211	1	6.922	406013	20.0
2-Pentanone, 4-...	5.151	20.9	ng	423635	1	6.922	406013	20.0
unknown7.069	7.069	2.2	ng	45541	1	6.922	406013	20.0
Ethanol, 2-(2-b...	8.110	8.2	ng	208489	2	8.210	507139	20.0
n-Hexadecanoic ...	11.975	2.7	ng	57597	4	11.457	426401	20.0
unknown14.027	14.027	4.8	ng	117911	5	14.110	488267	20.0
Triphenylphosph...	14.204	2.6	ng	63766	5	14.110	488267	20.0
Octadecane	15.245	3.0	ng	63614	6	15.621	422565	20.0
Benzo[e]pyrene	15.486	3.5	ng	73709	6	15.621	422565	20.0
Eicosane	16.104	3.3	ng	69684	6	15.621	422565	20.0
Heneicosane	16.639	2.1	ng	45057	6	15.621	422565	20.0