LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140191.D
Acq On : 31 Oct 2024 16:08
Operator : RC/JU
Sample : P4614-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-07-102924

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	6	13	rVB	731225	1110518	56.01%	6.586%
2	5.499	573	579	584	rBV	1340462	1767065	89.13%	10.479%
3	6.504	744	750	755	rBV	1370089	1789848	90.28%	10.614%
4	6.881	809	814	820	rBV	487479	603351	30.43%	3.578%
5	7.440	901	909	914	rBV	939286	1199606	60.51%	7.114%
6	7.693	948	952	959	rVB	31936	40034	2.02%	0.237%
7	8.163	1024	1032	1040	rBV	634469	779143	39.30%	4.621%
8	8.375	1063	1068	1074	rVB	16431	20751	1.05%	0.123%
9	9.239	1210	1215	1220	rBV	1622849	1982579	100.00%	11.757%
10	9.851	1313	1319	1323	rBV2	12007	20273	1.02%	0.120%
11	9.922	1326	1331	1336	rBV	603950	754104	38.04%	4.472%
12	10.086	1354	1359	1362	rBV2	12244	21174	1.07%	0.126%
13	10.351	1398	1404	1408	rBV2	19195	28213	1.42%	0.167%
14	10.569	1436	1441	1448	rBV	14877	33897	1.71%	0.201%
15	10.639	1448	1453	1459	rVB	283819	357697	18.04%	2.121%
16	10.710	1460	1465	1472	rBV	751385	1010268	50.96%	5.991%
17	10.833	1481	1486	1493	rBV2	28352	59662	3.01%	0.354%
18	10.951	1502	1506	1510	rVB	35342	45217	2.28%	0.268%
19	11.028	1514	1519	1522	rBV	30021	52260	2.64%	0.310%
20	11.157	1537	1541	1547	rVB3	14115	20454	1.03%	0.121%
21	11.281	1557	1562	1565	rBV	31432	46206	2.33%	0.274%
22	11.310	1565	1567	1572	rVB2	19289	22704	1.15%	0.135%
23	11.416	1580	1585	1594	rBV2	542567	811823	40.95%	4.814%
24	11.492	1594	1598	1601	rVB	20263	27372	1.38%	0.162%
25	11.945	1667	1675	1686	rBV	362166	574737	28.99%	3.408%
26	12.033	1686	1690	1698	rVB2	31132	64026	3.23%	0.380%
27	12.116	1701	1704	1709	rBV3	21045	28207	1.42%	0.167%
28	12.510	1768	1771	1776	rVB2	22304	30478	1.54%	0.181%
29	12.633	1788	1792	1805	rBV	247181	367056	18.51%	2.177%
30	12.733	1805	1809	1816	rBV	113220	190574	9.61%	1.130%
31	12.863	1826	1831	1838	rBV	193932	285023	14.38%	1.690%
32	13.010	1851	1856	1863	rVB	1207828	1547303	78.04%	9.176%
33	13.927	2008	2012	2021	rVB3	84450	155424	7.84%	0.922%
34	14.080	2032	2038	2049	rBV2	395860	723848	36.51%	4.293%
35	15.610	2294	2298	2302	rBV	197709	291613	14.71%	1.729%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140191.D
Acq On : 31 Oct 2024 16:08
Operator : RC/JU
Sample : P4614-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-07-102924

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

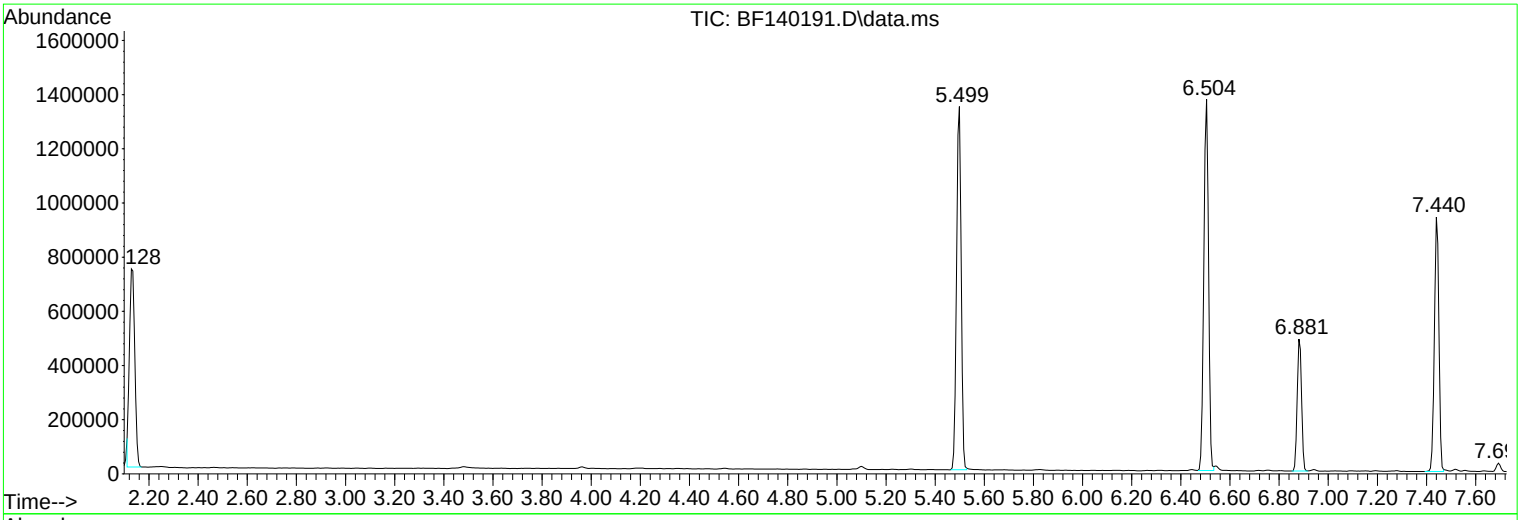
Sum of corrected areas: 16862508

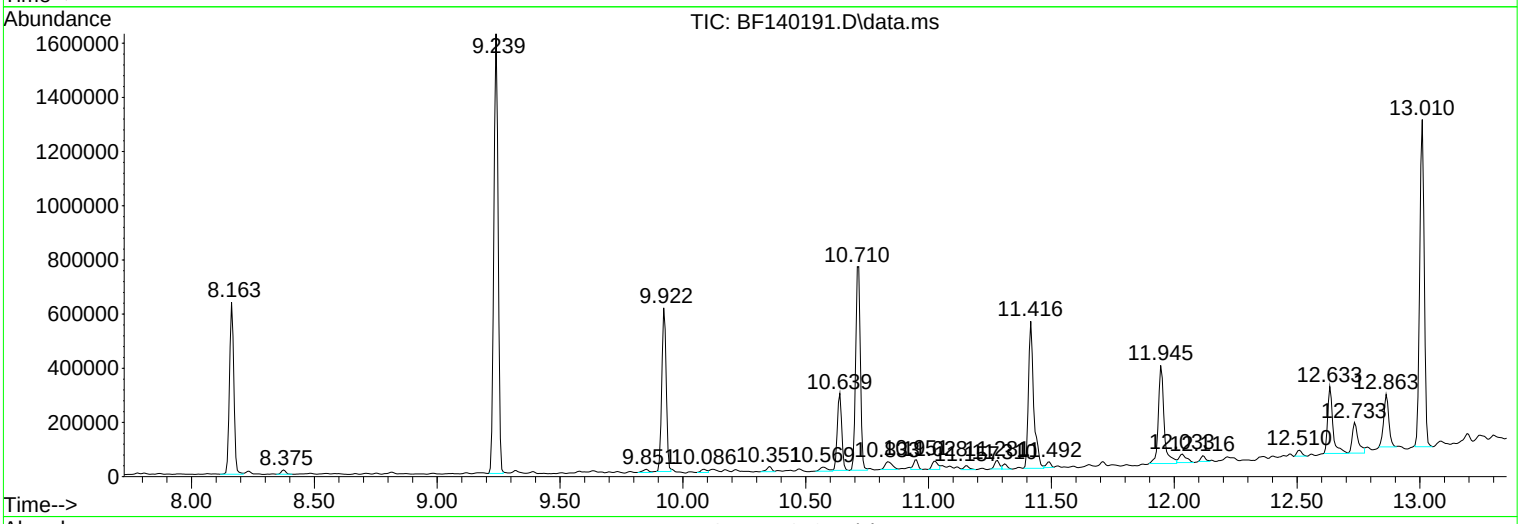
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140191.D
Acq On : 31 Oct 2024 16:08
Operator : RC/JU
Sample : P4614-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

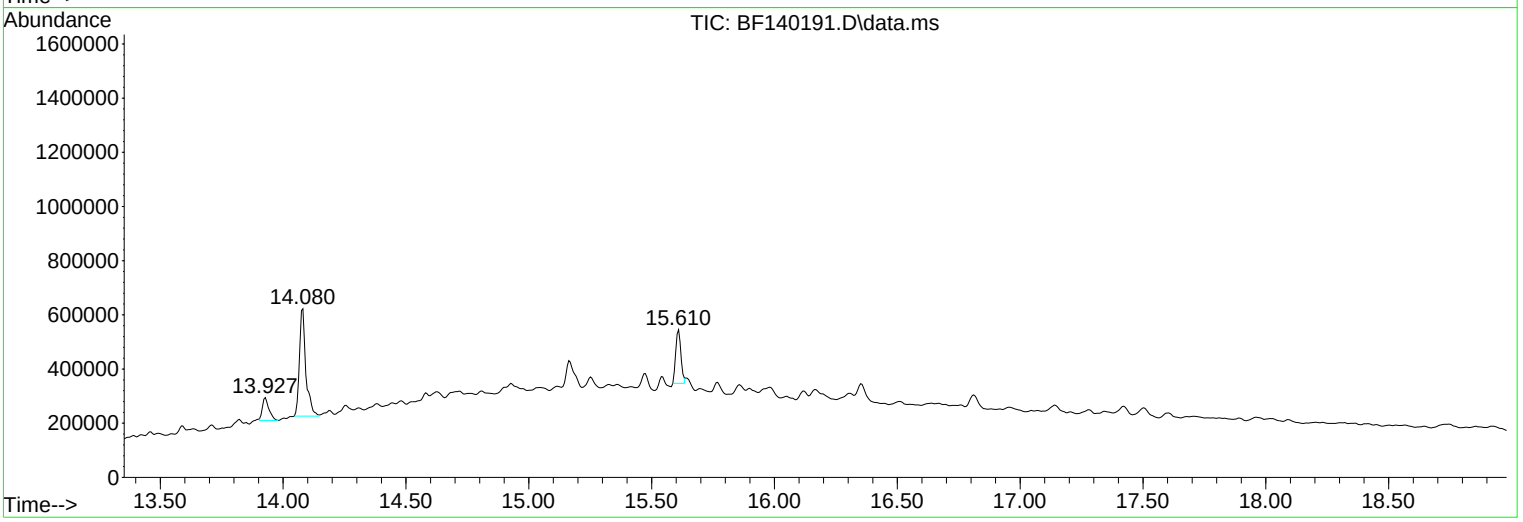
Instrument :
BNA_F
ClientSampleId :
NB-07-102924

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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 : BF140191.D
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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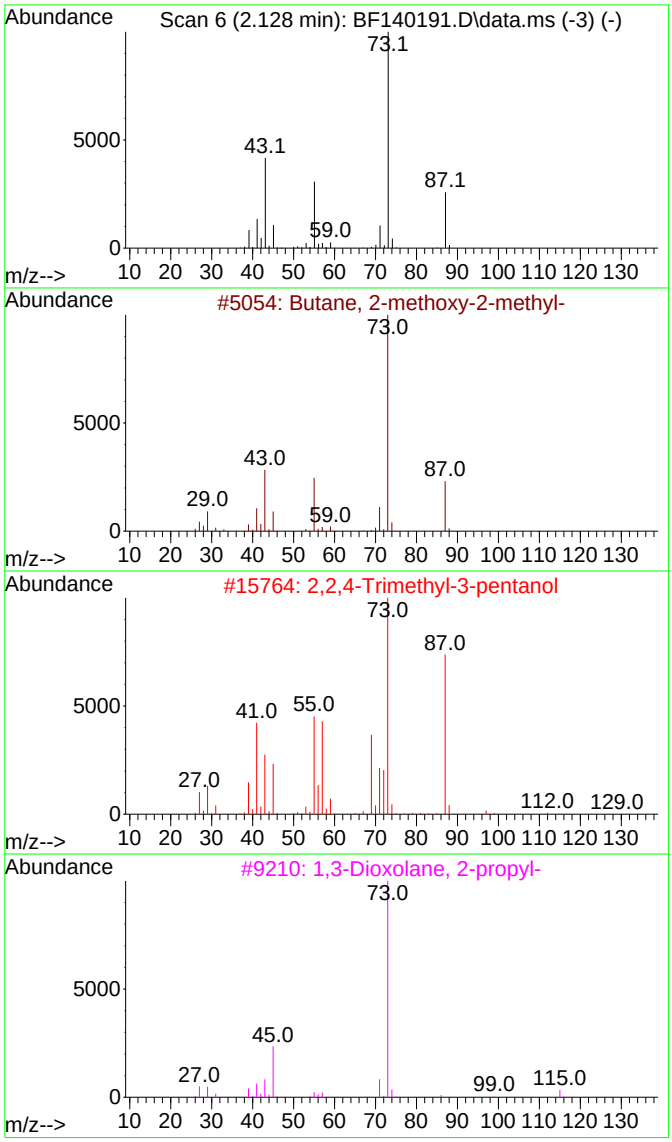
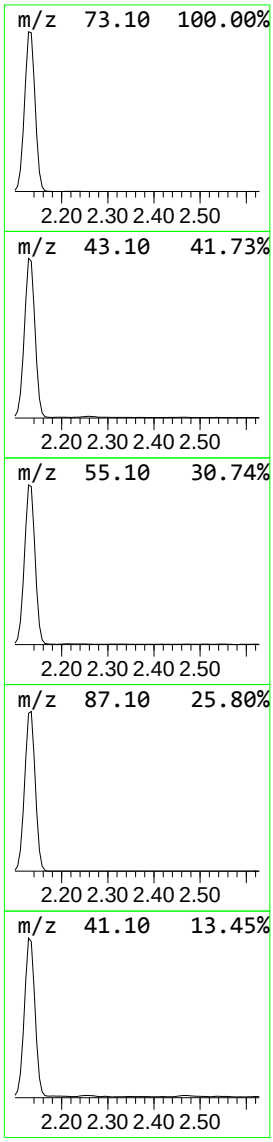
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	36.81 ng	1110520	1,4-Dichlorobenzene-d4	6.881

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	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140191.D
Acq On : 31 Oct 2024 16:08
Operator : RC/JU
Sample : P4614-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-07-102924

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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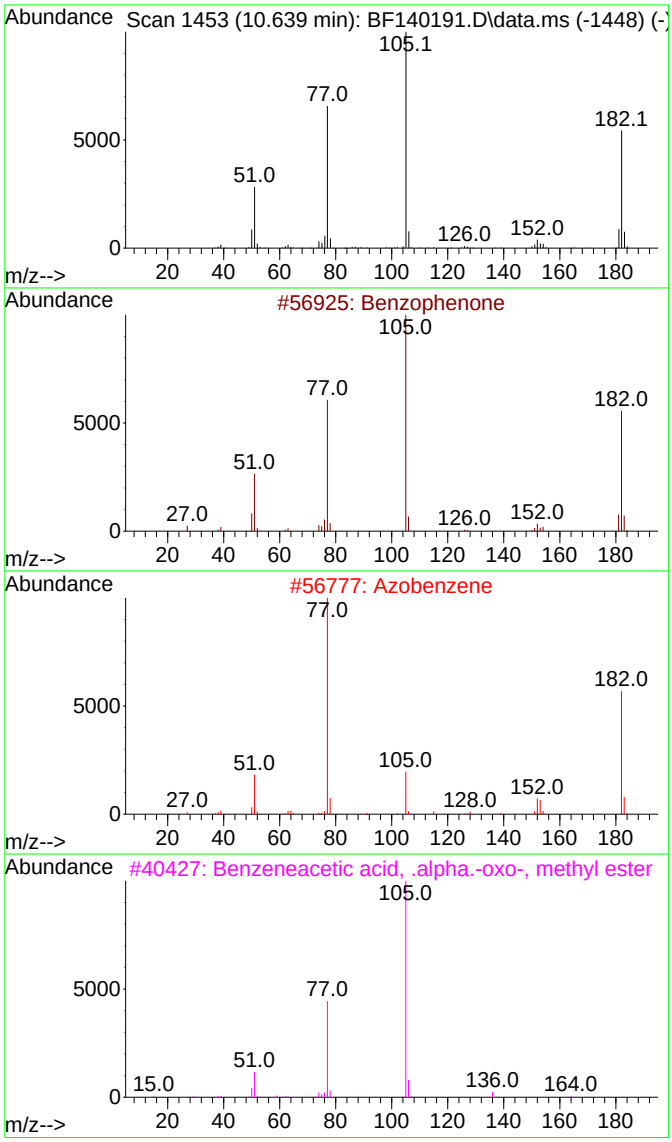
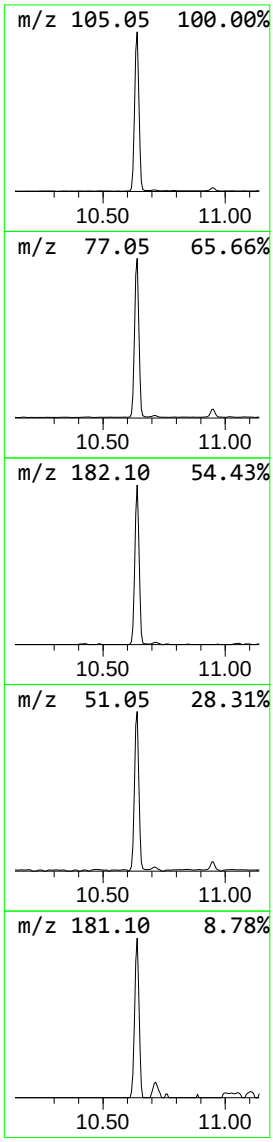
Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	9.49 ng	357697	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
4	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140191.D
Acq On : 31 Oct 2024 16:08
Operator : RC/JU
Sample : P4614-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-07-102924

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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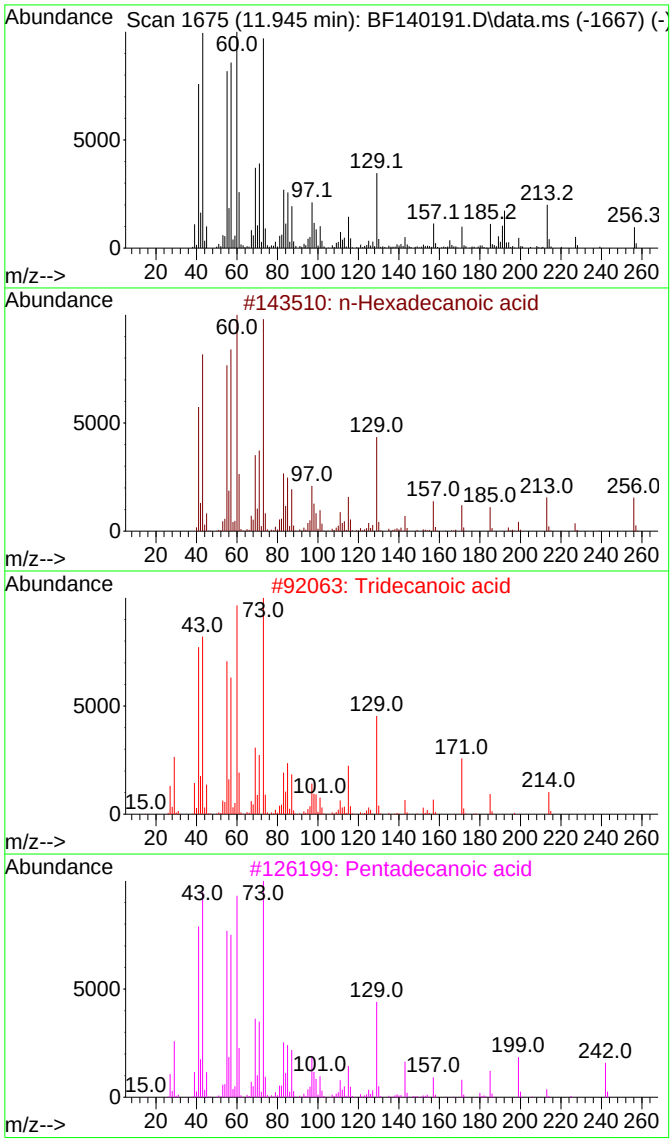
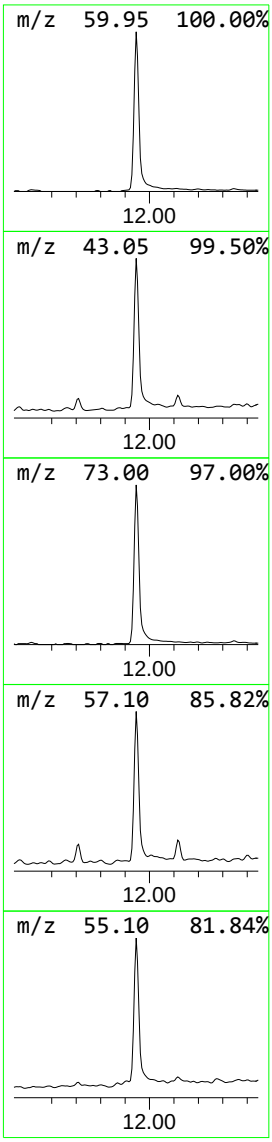
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	14.16 ng	574737	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140191.D
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Operator : RC/JU
Sample : P4614-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-07-102924

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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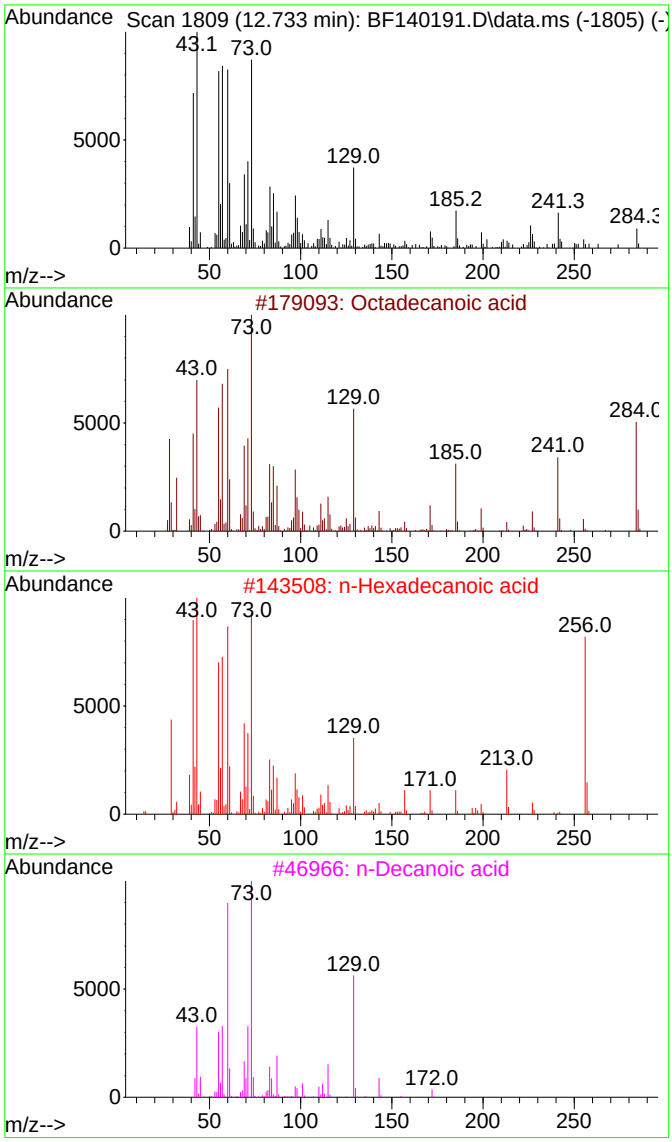
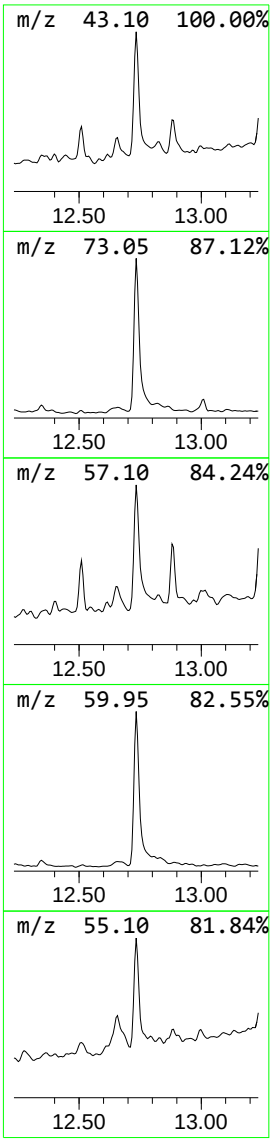
Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	4.69 ng	190574	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	n-Decanoic acid	172	C10H20O2	000334-48-5	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
Data File : BF140191.D
Acq On : 31 Oct 2024 16:08
Operator : RC/JU
Sample : P4614-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-07-102924

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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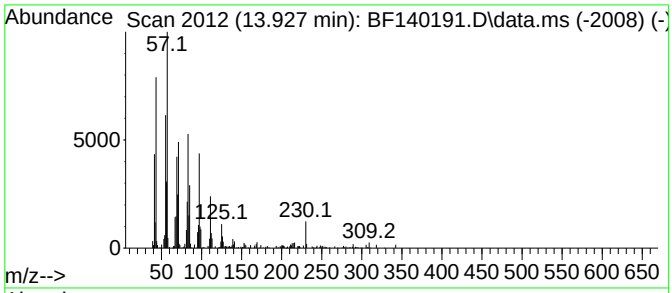
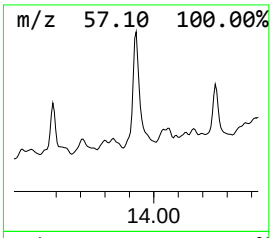
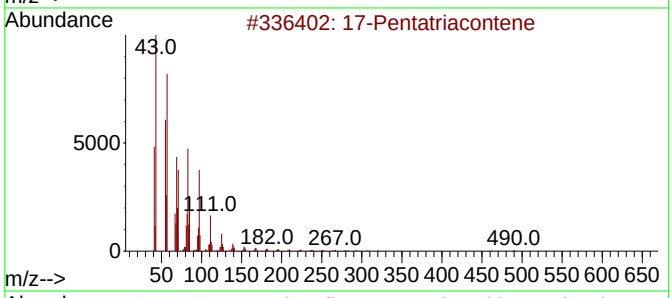
Peak Number 5 17-Pentatriacontene Concentration Rank 5

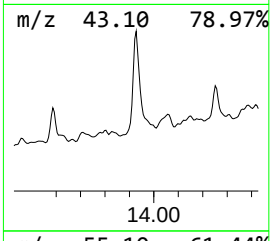
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	4.29 ng	155424	Chrysene-d12	14.080

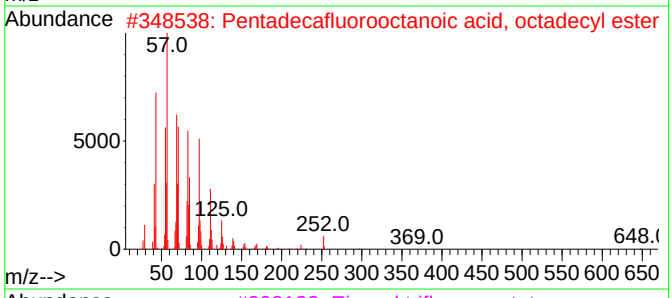
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	94
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91

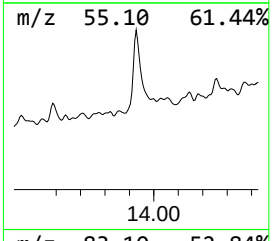


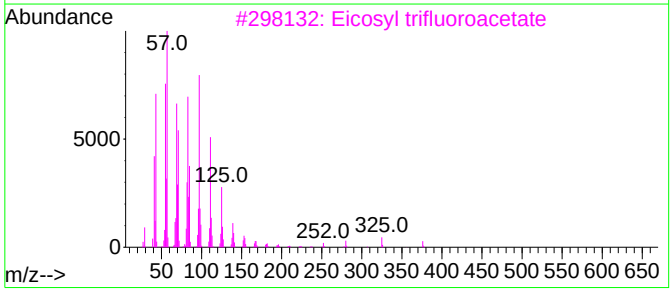


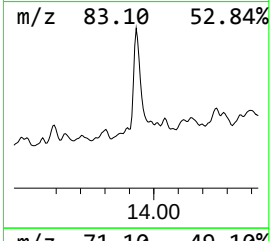


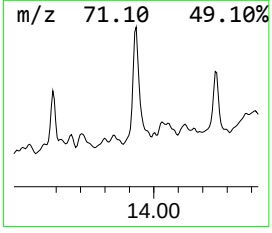












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103124\
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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...	2.128	36.8	ng	1110520	1	6.881	603351	20.0
Benzophenone	10.639	9.5	ng	357697	3	9.922	754104	20.0
n-Hexadecanoic ...	11.945	14.2	ng	574737	4	11.416	811823	20.0
Octadecanoic acid	12.733	4.7	ng	190574	4	11.416	811823	20.0
17-Pentatriacon...	13.927	4.3	ng	155424	5	14.080	723848	20.0