LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138889.D
Acq On : 09 Aug 2024 15:31
Operator : RC/JU
Sample : P3468-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-682-697

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138889.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	5	11	rVB	2035083	2490446	100.00%	20.365%
2	3.899	301	307	319	rBB	107348	173255	6.96%	1.417%
3	5.057	499	504	516	rVB	30746	45290	1.82%	0.370%
4	5.469	569	574	589	rBV	477199	644241	25.87%	5.268%
5	5.787	624	628	636	rBV	30300	45179	1.81%	0.369%
6	6.481	741	746	759	rBV	289229	403331	16.20%	3.298%
7	6.840	802	807	813	rBV	217744	272152	10.93%	2.225%
8	7.404	897	903	908	rBV	789160	1066745	42.83%	8.723%
9	8.116	1019	1024	1030	rBV	282301	362048	14.54%	2.961%
10	9.192	1201	1207	1212	rBV	1517892	1941439	77.96%	15.876%
11	9.869	1317	1322	1332	rBV	339766	423969	17.02%	3.467%
12	9.963	1332	1338	1345	rBV	111969	172419	6.92%	1.410%
13	10.663	1452	1457	1472	rBV	675656	880634	35.36%	7.201%
14	11.357	1570	1575	1583	rBV	375103	465160	18.68%	3.804%
15	12.445	1746	1760	1772	rBV3	22102	75821	3.04%	0.620%
16	12.569	1776	1781	1785	rBV	27511	43566	1.75%	0.356%
17	12.616	1785	1789	1793	rVV3	16877	25053	1.01%	0.205%
18	12.686	1797	1801	1808	rVB2	40540	61147	2.46%	0.500%
19	12.804	1814	1821	1826	rBV2	13929	28749	1.15%	0.235%
20	12.945	1839	1845	1850	rVB	1526711	2049187	82.28%	16.757%
21	13.963	2014	2018	2020	rBV	26571	30772	1.24%	0.252%
22	13.998	2020	2024	2034	rVB	206950	265950	10.68%	2.175%
23	14.821	2160	2164	2169	rBV	29084	41111	1.65%	0.336%
24	15.463	2267	2273	2285	rBV	135612	221389	8.89%	1.810%

Sum of corrected areas: 12229053

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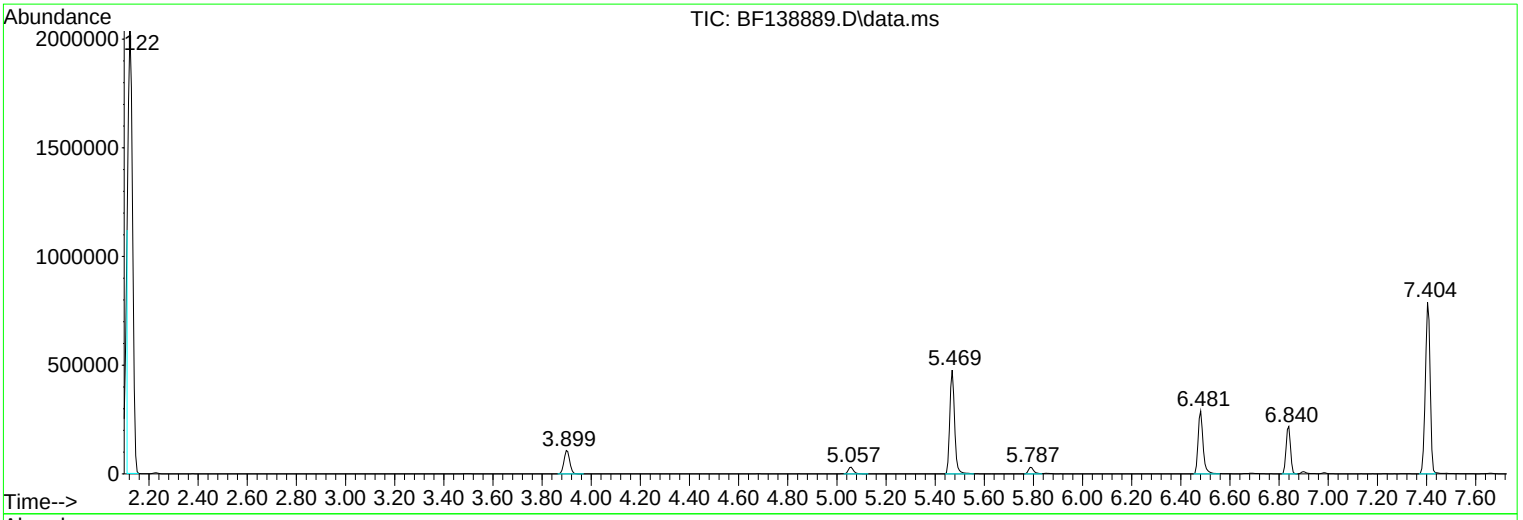
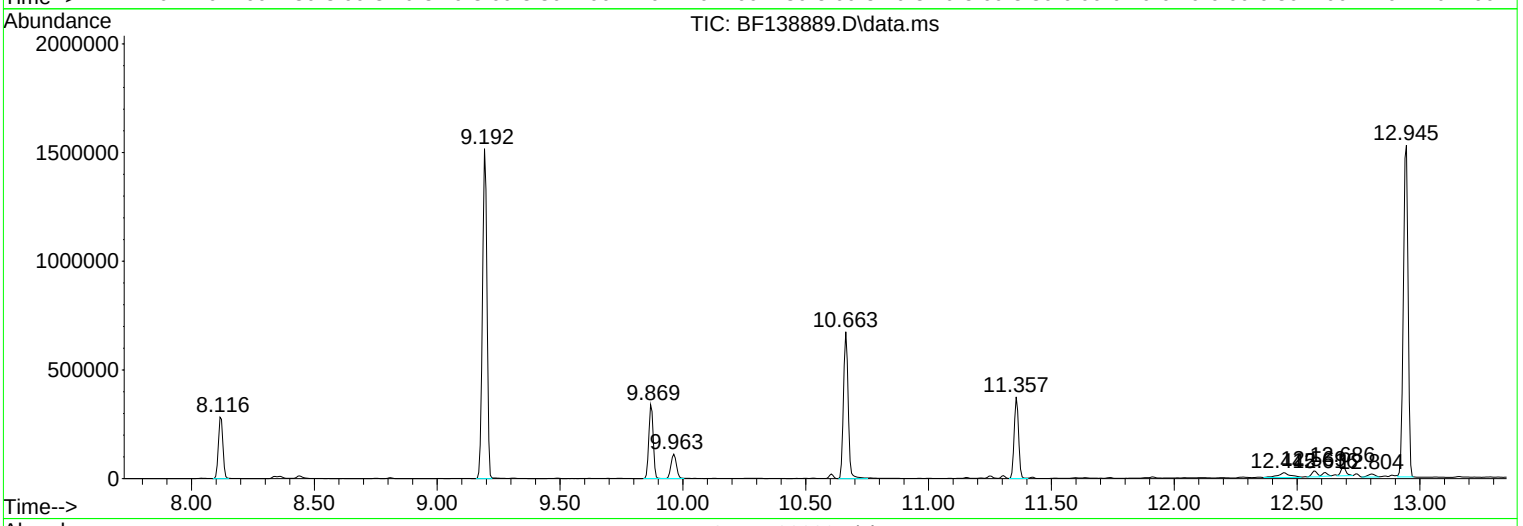
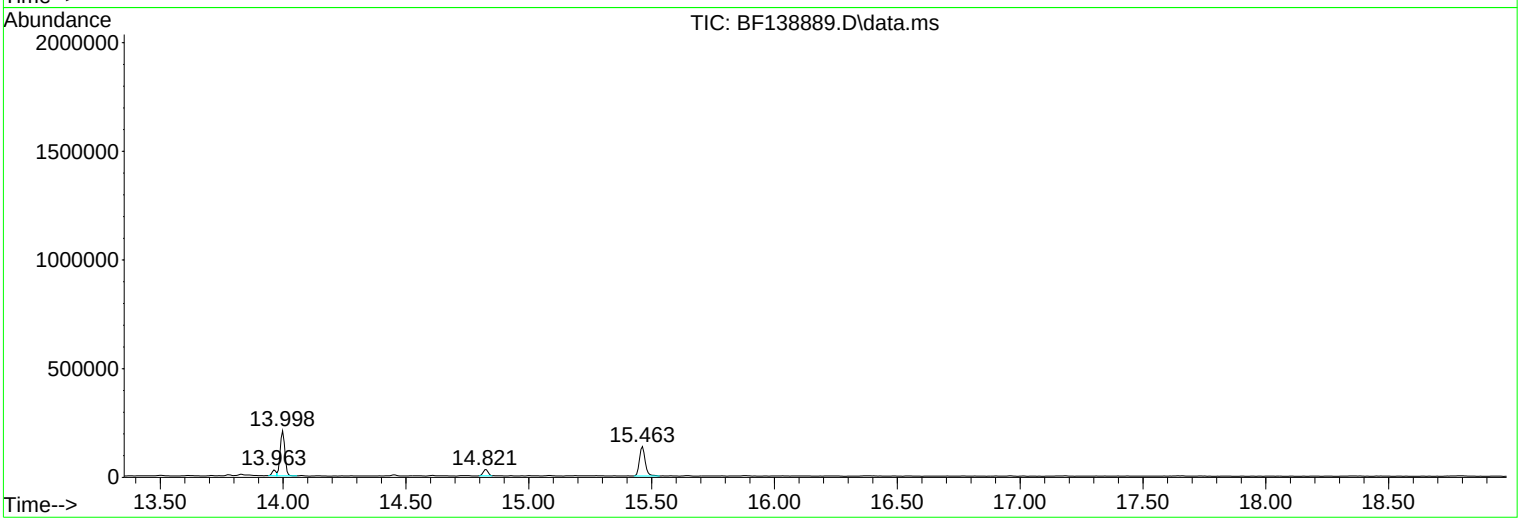
ClientSampleId :
MLS-15-682-697

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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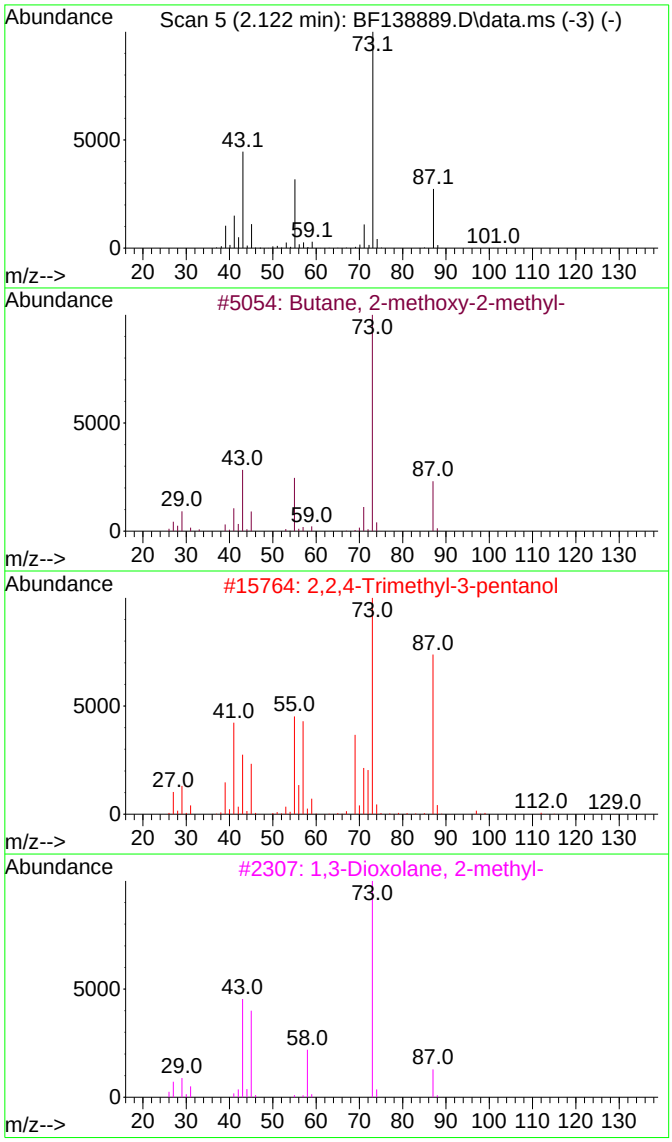
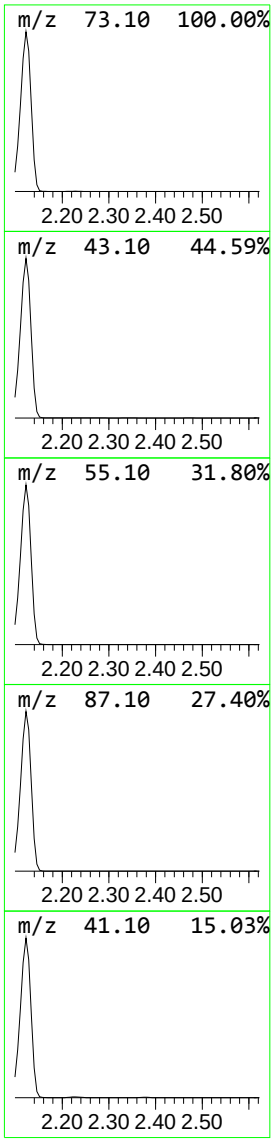
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	183.02 ng	2490450	1,4-Dichlorobenzene-d4	6.840

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-methyl-	88	C4H8O2	000497-26-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Operator : RC/JU
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MLS-15-682-697

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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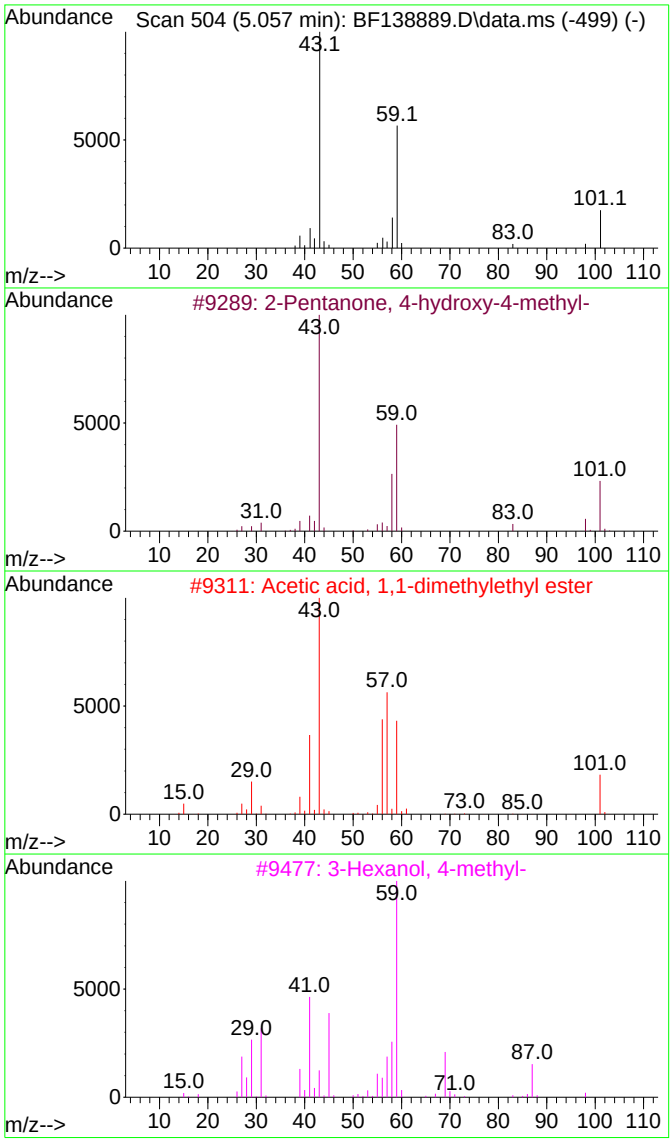
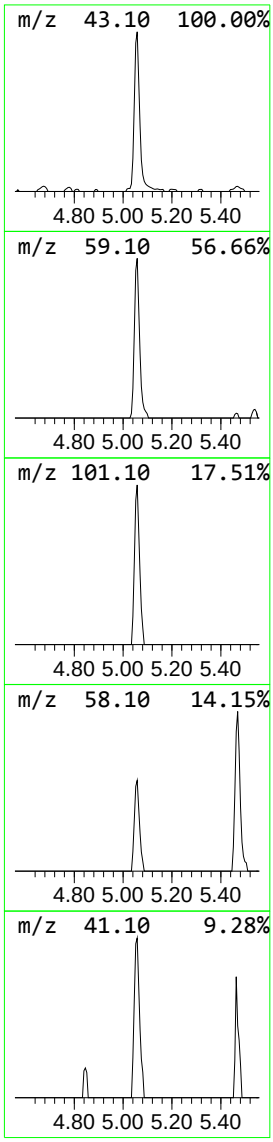
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	3.33 ng	45290	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	23





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Instrument :
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ClientSampleId :
MLS-15-682-697

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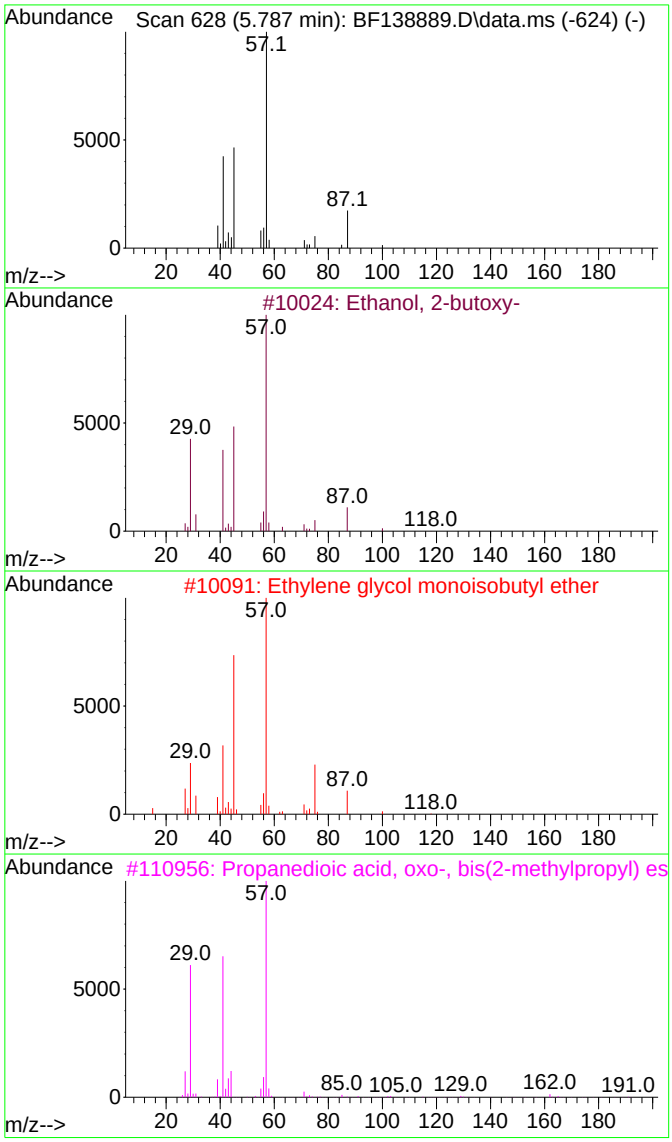
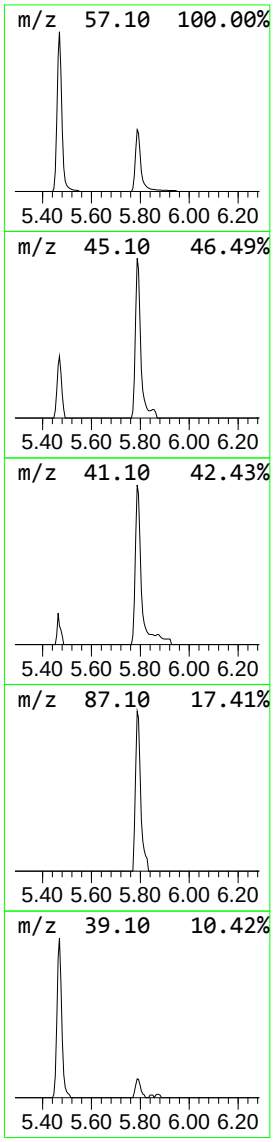
Peak Number 4 Ethanol, 2-butoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.787	3.32 ng	45179	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	56
3	Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	12
4	1-Penten-3-ol, 4-methyl-	100	C6H12O	004798-45-2	12
5	1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	12





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-682-697

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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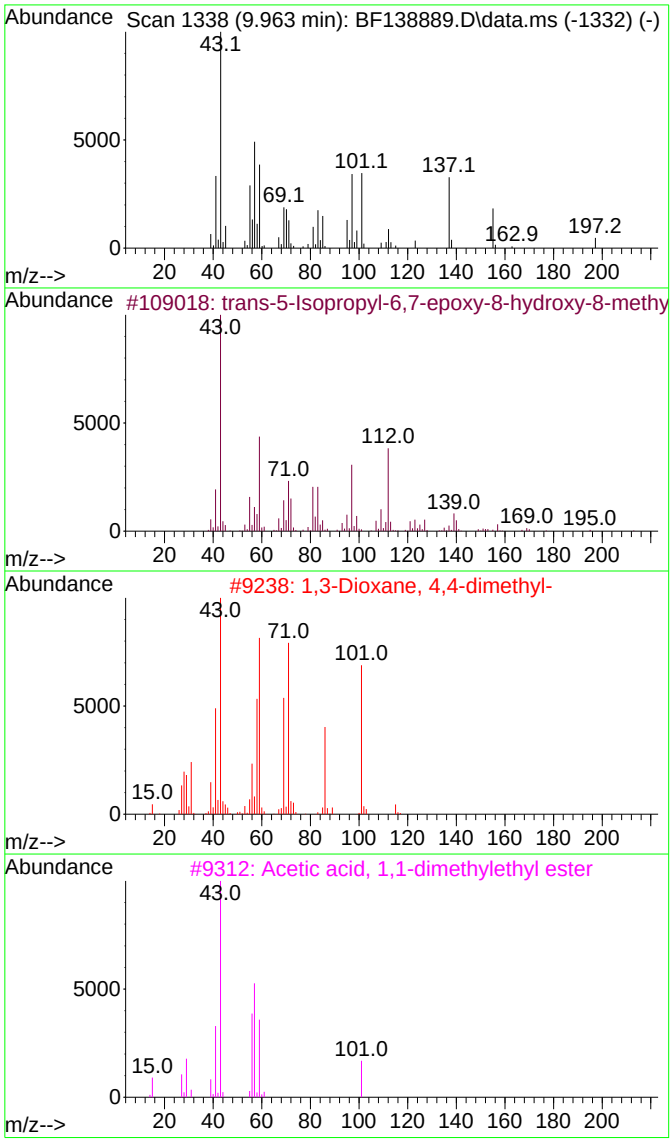
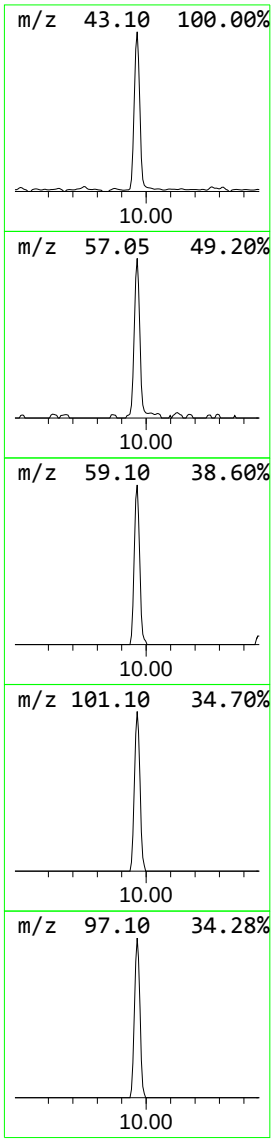
****

Peak Number 5 unknown9.963 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.963	8.13 ng	172419	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	32
2	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	27
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	16
4	3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	16
5	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	14





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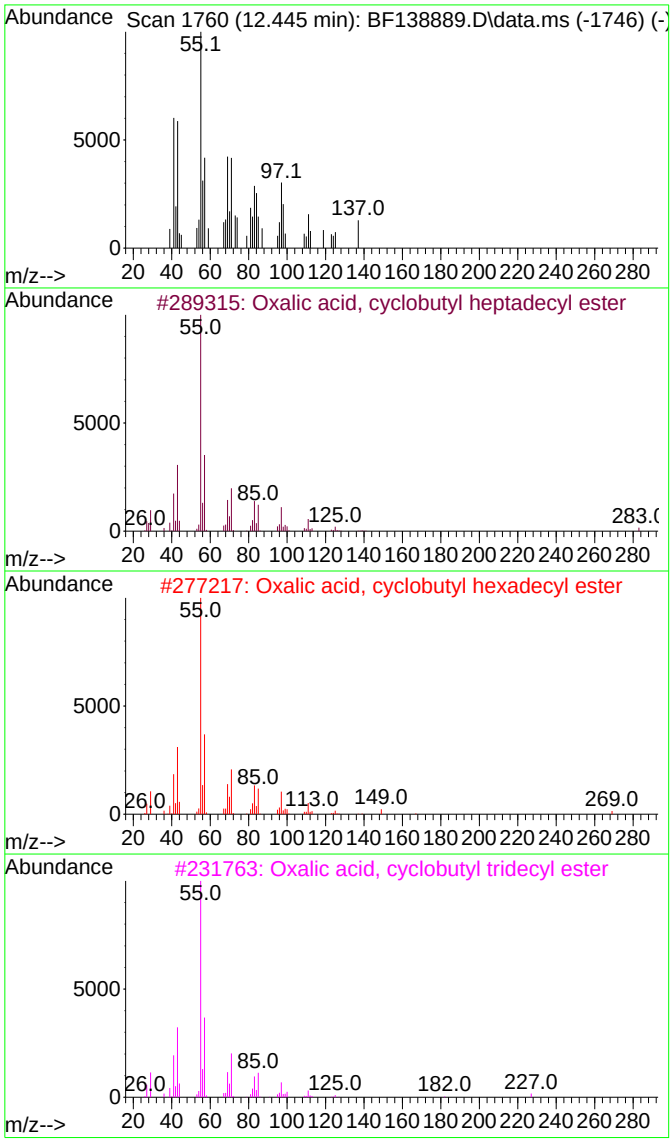
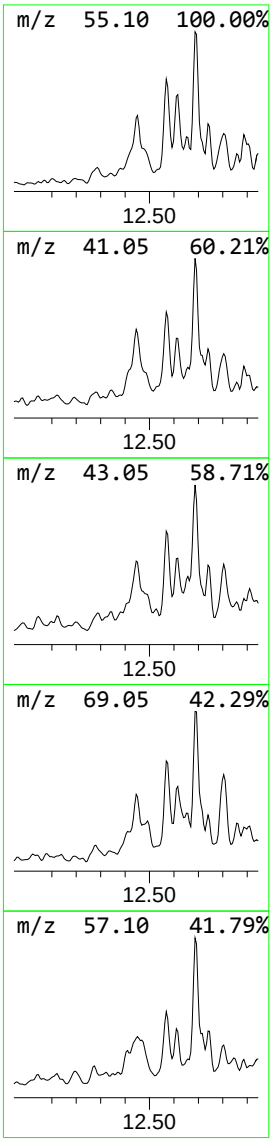
Peak Number 6 Oxalic acid, cyclobutyl hep... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	3.26 ng	75821	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	52
2	Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	50
3	Oxalic acid, cyclobutyl tridecyl...	326	C19H34O4	1000309-70-4	43
4	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1010282-97-2	43
5	Ethylene diacrylate	170	C8H10O4	002274-11-5	38





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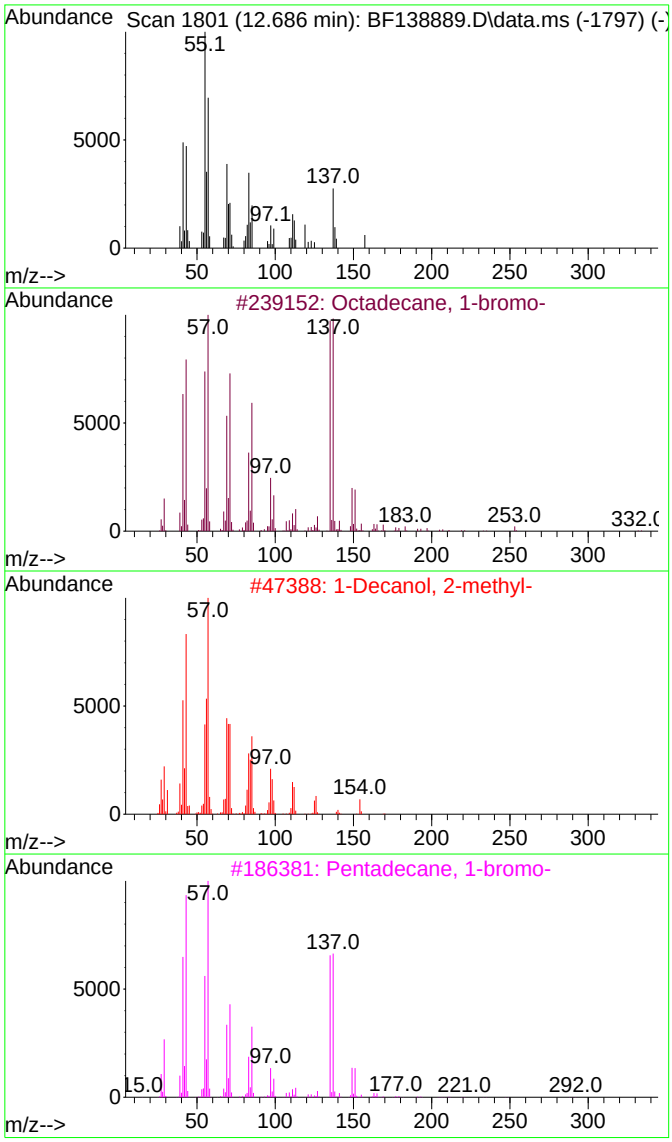
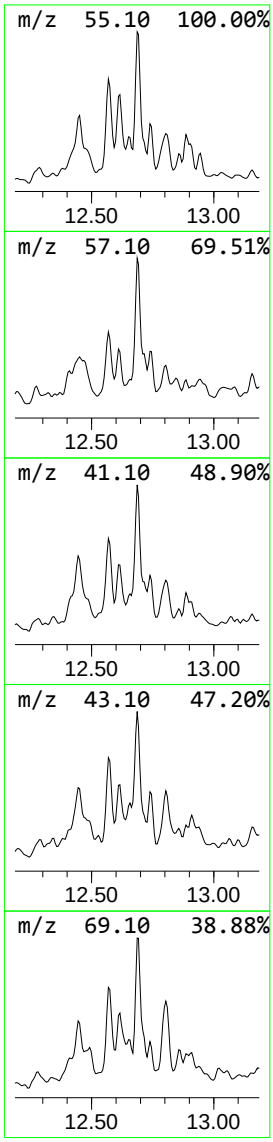
Peak Number 7 unknown12.686 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	4.60 ng	61147	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	47
2	1-Decanol, 2-methyl-	172	C11H24O	018675-24-6	43
3	Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	43
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	38
5	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	35





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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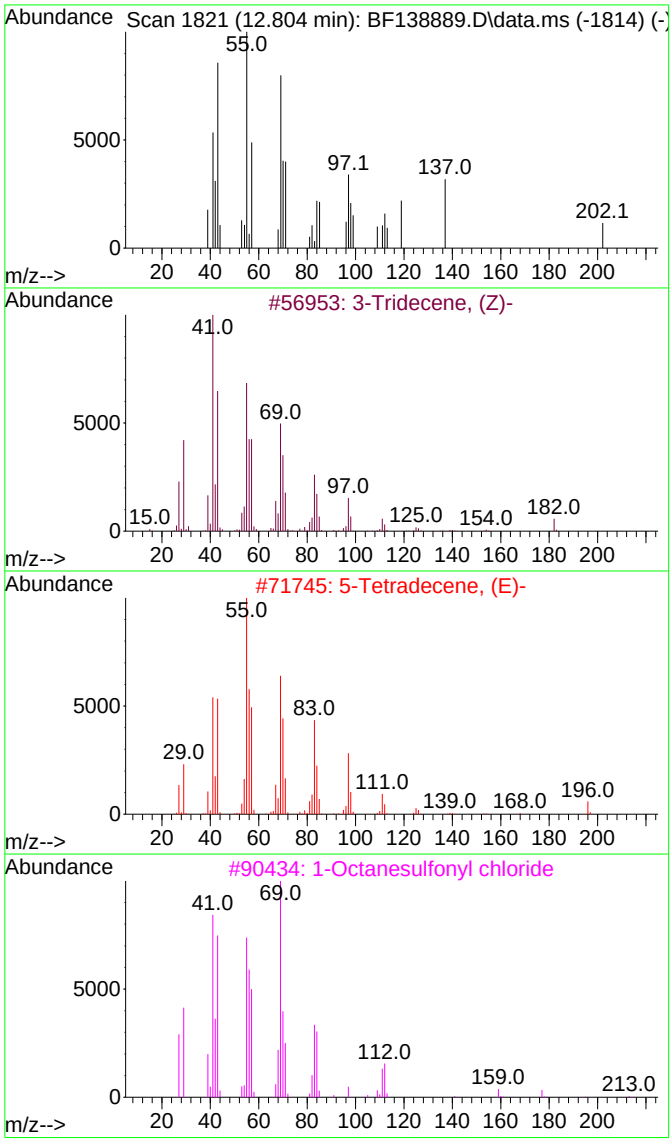
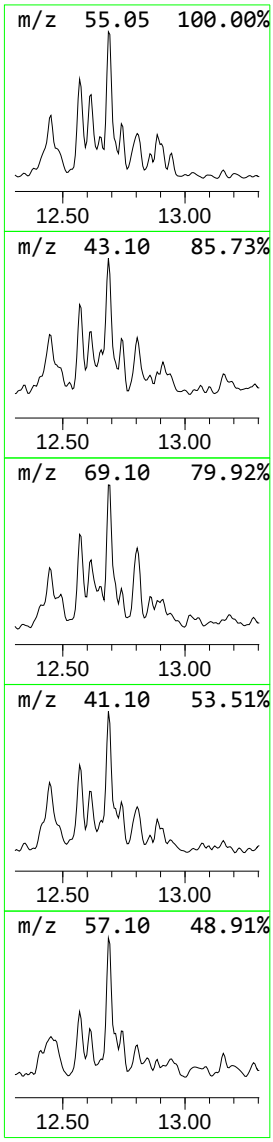
Peak Number 8 3-Tridecene, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.804	2.16 ng	28749	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Tridecene, (Z)-	182	C13H26	041446-53-1	50
2	5-Tetradecene, (E)-	196	C14H28	041446-66-6	47
3	1-Octanesulfonyl chloride	212	C8H17ClO2S	007795-95-1	38
4	Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	38
5	Diphosphoric acid, diisooctyl ester	402	C16H36O7P2	072101-07-6	35





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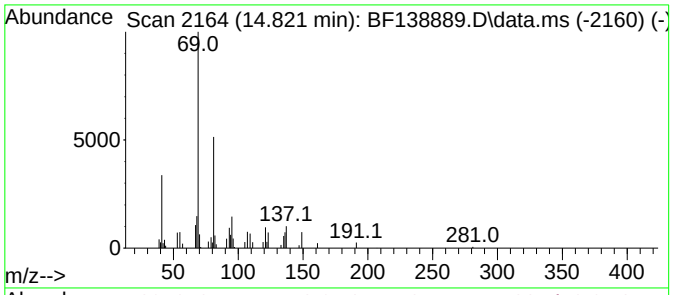
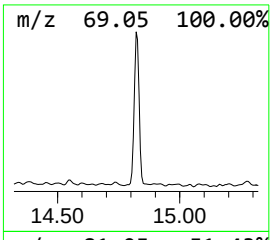
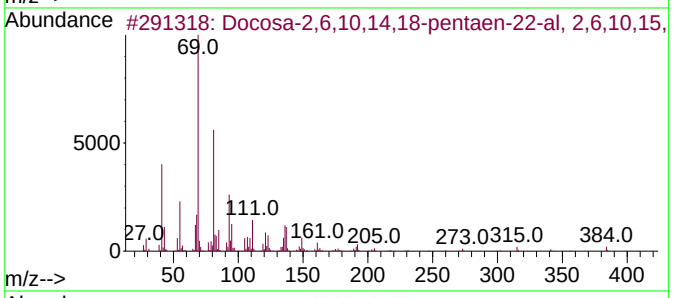
Peak Number 9 Docosa-2,6,10,14,18-pentaen... Concentration Rank 5

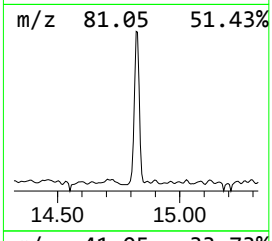
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	3.71 ng	41111	Perylene-d12	15.463

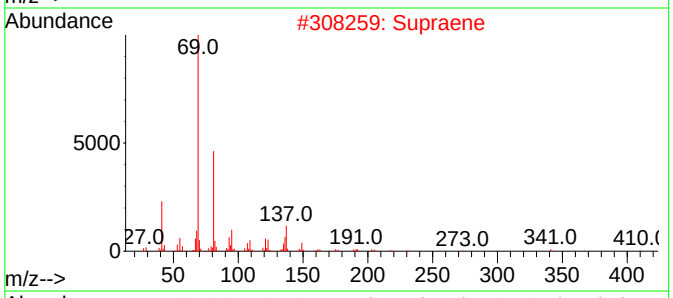
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
2	Supraene	410	C30H50	007683-64-9	90
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	86
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72

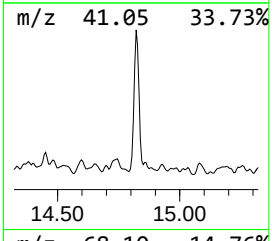


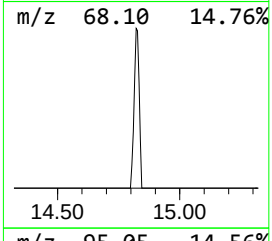


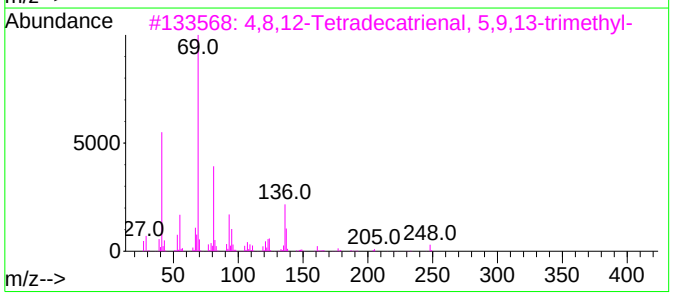


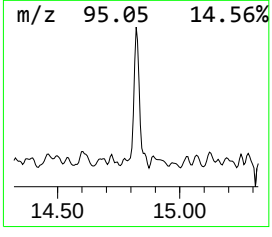












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138889.D
Acq On : 09 Aug 2024 15:31
Operator : RC/JU
Sample : P3468-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-682-697

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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...	2.122	183.0	ng	2490450	1	6.840	272152	20.0
2-Pentanone, 4-...	5.057	3.3	ng	45290	1	6.840	272152	20.0
Ethanol, 2-butoxy-	5.787	3.3	ng	45179	1	6.840	272152	20.0
unknown9.963	9.963	8.1	ng	172419	3	9.869	423969	20.0
Oxalic acid, cy...	12.445	3.3	ng	75821	4	11.357	465160	20.0
unknown12.686	12.686	4.6	ng	61147	5	13.998	265950	20.0
3-Tridecene, (Z)-	12.804	2.2	ng	28749	5	13.998	265950	20.0
Docosa-2,6,10,1...	14.821	3.7	ng	41111	6	15.463	221389	20.0