

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072924\
 Data File : BF138678.D
 Acq On : 29 Jul 2024 19:47
 Operator : RC/JU
 Sample : P3367-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-06-07252024

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-BF070924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138678.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	20	rVB	1685331	2611211	100.00%	15.185%
2	3.387	215	220	236	rBV	16096	64618	2.47%	0.376%
3	5.075	502	507	517	rVB	103523	162360	6.22%	0.944%
4	5.481	570	576	591	rVB	1583860	2096291	80.28%	12.190%
5	6.487	741	747	763	rBV	1571894	2117427	81.09%	12.313%
6	6.845	803	808	814	rVB	478697	604702	23.16%	3.516%
7	7.410	898	904	909	rBV	1010066	1321656	50.61%	7.686%
8	7.663	941	947	953	rVB	32260	40607	1.56%	0.236%
9	8.128	1017	1026	1033	rBV	573544	722812	27.68%	4.203%
10	8.445	1068	1080	1088	rBV	50092	82829	3.17%	0.482%
11	9.210	1204	1210	1215	rBV	1489417	1879214	71.97%	10.928%
12	9.886	1320	1325	1330	rBV	483132	591844	22.67%	3.442%
13	9.980	1336	1341	1346	rVB2	33868	52922	2.03%	0.308%
14	10.680	1454	1460	1474	rBV	631868	843998	32.32%	4.908%
15	10.798	1474	1480	1488	rVB2	21364	40925	1.57%	0.238%
16	11.374	1573	1578	1586	rBV	421352	575300	22.03%	3.345%
17	11.763	1640	1644	1648	rBV	27334	35790	1.37%	0.208%
18	11.904	1660	1668	1674	rBV3	55011	103232	3.95%	0.600%
19	11.986	1679	1682	1690	rVB3	21610	43419	1.66%	0.252%
20	12.069	1692	1696	1700	rBV2	18479	26627	1.02%	0.155%
21	12.451	1753	1761	1769	rBV4	110826	267147	10.23%	1.554%
22	12.586	1781	1784	1789	rVB	115751	147540	5.65%	0.858%
23	12.821	1818	1824	1829	rBV	119772	200319	7.67%	1.165%
24	12.963	1842	1848	1856	rVB	1160902	1519420	58.19%	8.836%
25	13.186	1883	1886	1893	rBV4	21120	41385	1.58%	0.241%
26	13.863	1997	2001	2010	rVB	83936	154664	5.92%	0.899%
27	14.015	2022	2027	2038	rVB2	311624	515025	19.72%	2.995%
28	15.486	2273	2277	2293	rVB	190685	333080	12.76%	1.937%

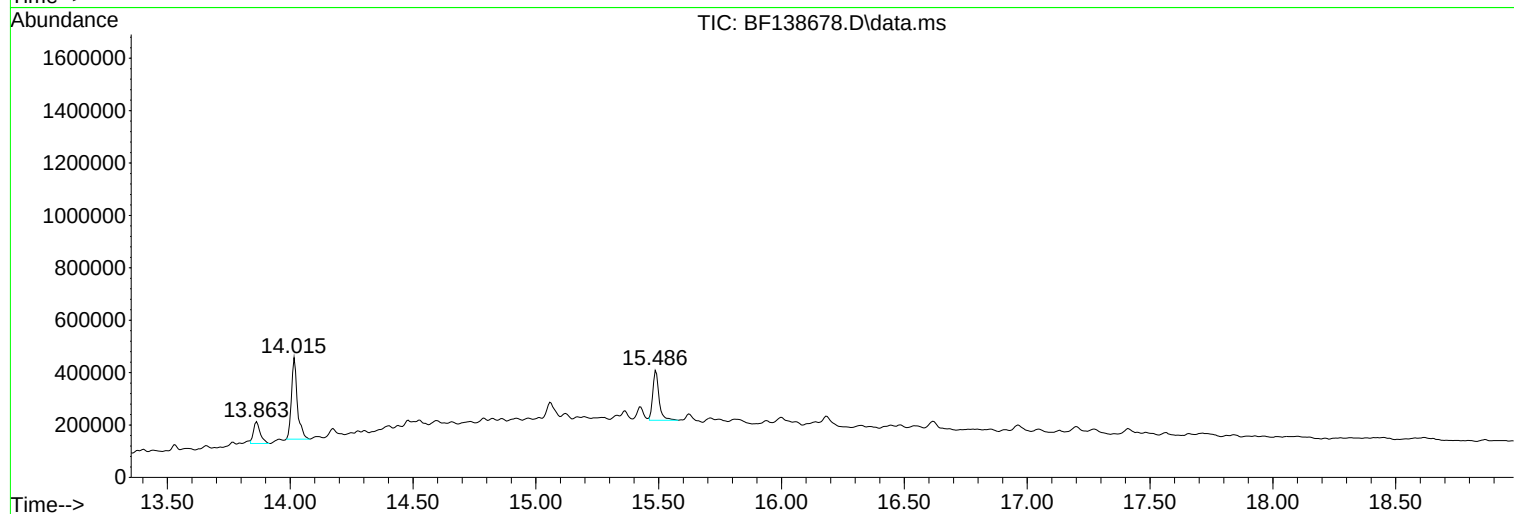
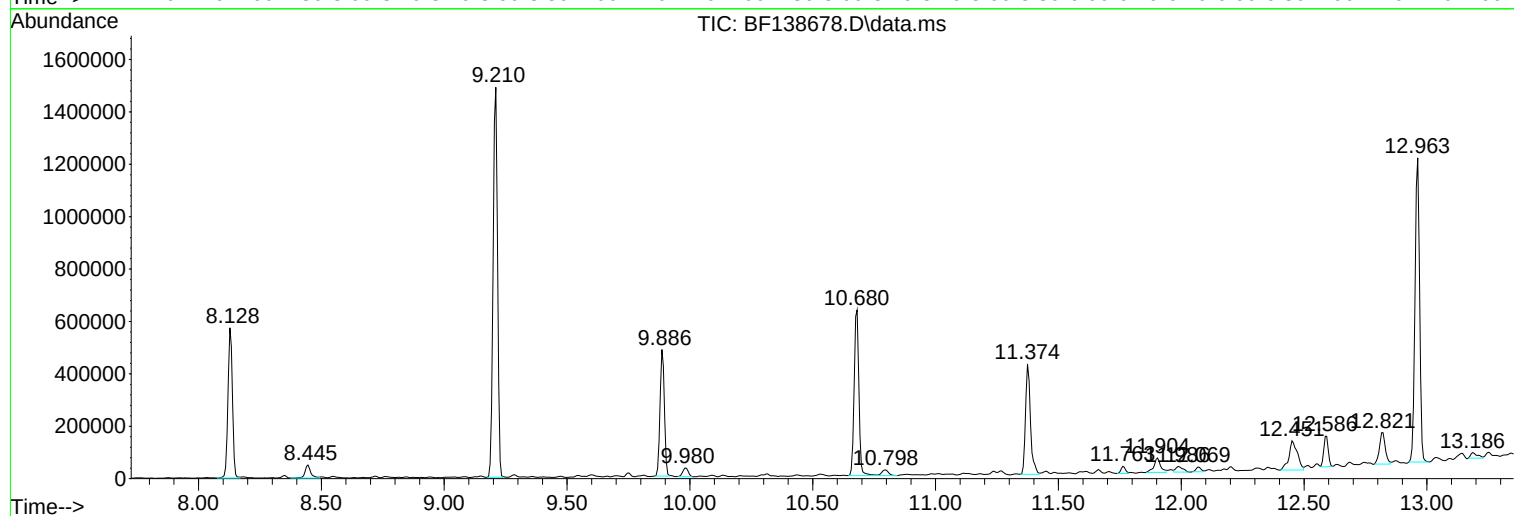
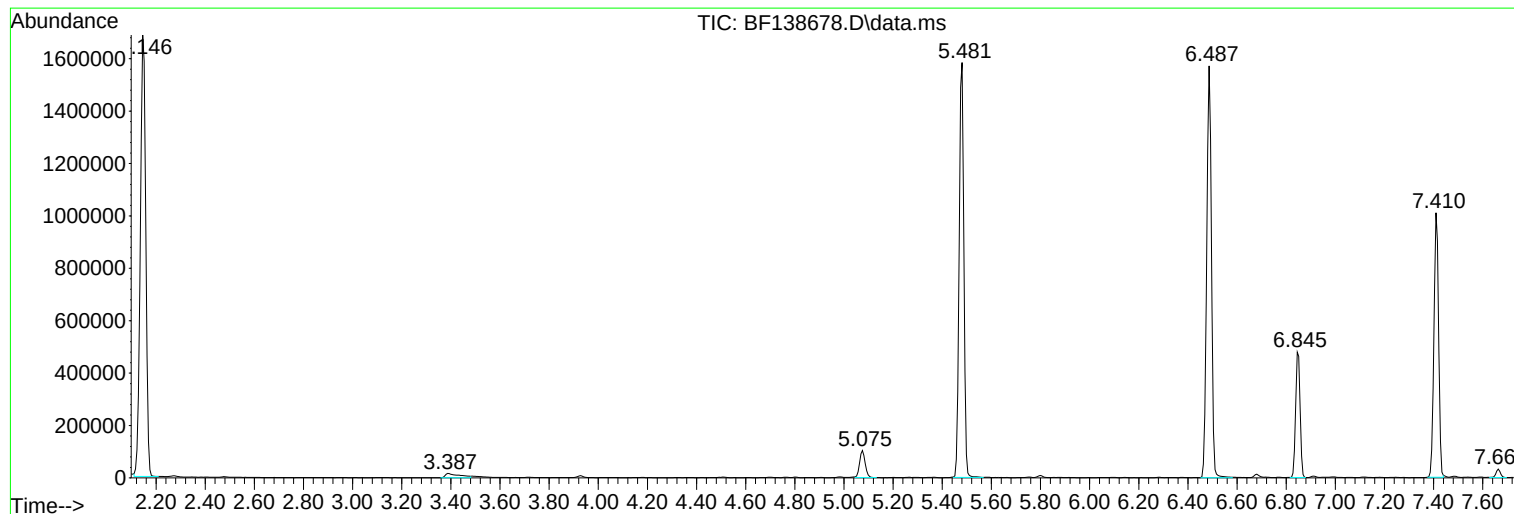
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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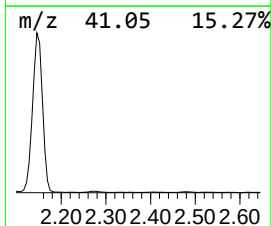
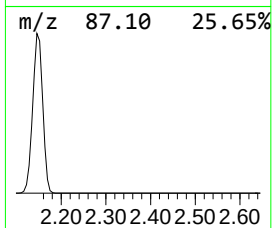
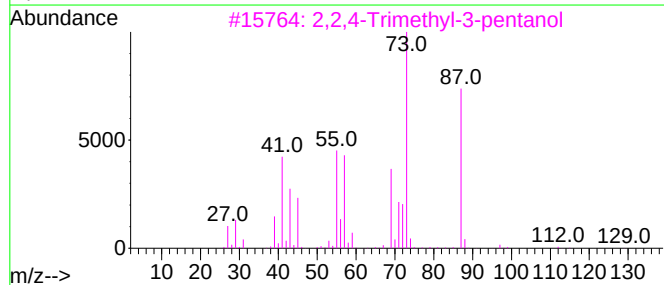
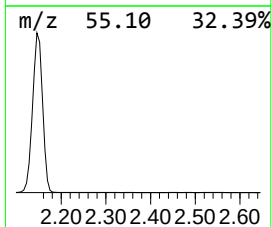
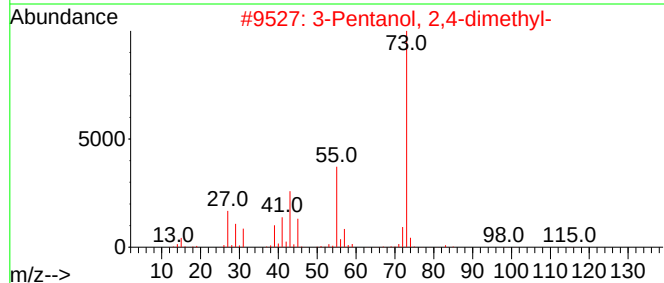
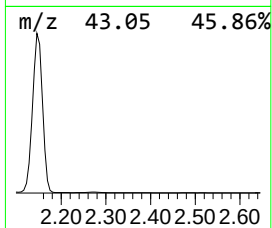
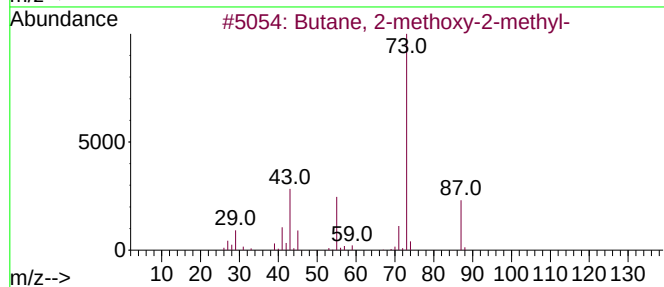
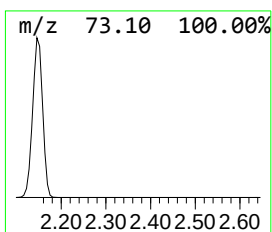
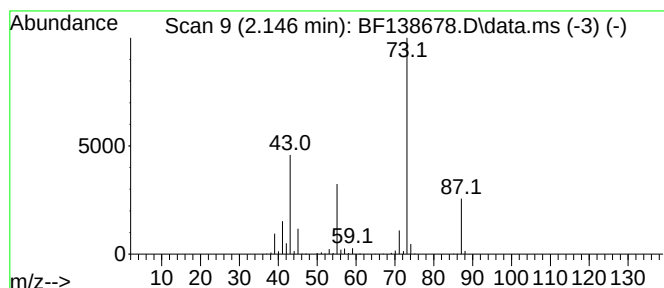
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.146	86.36 ng	2611210	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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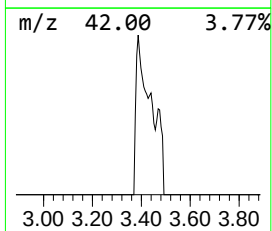
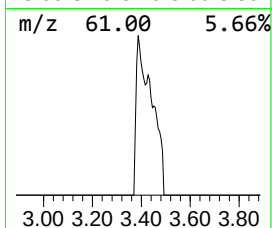
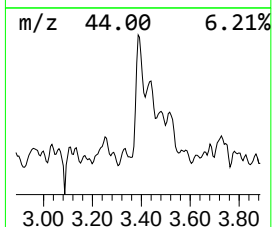
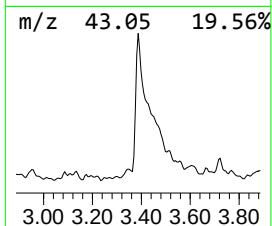
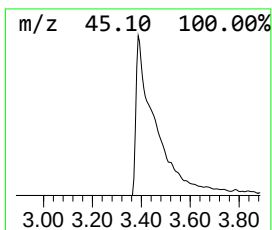
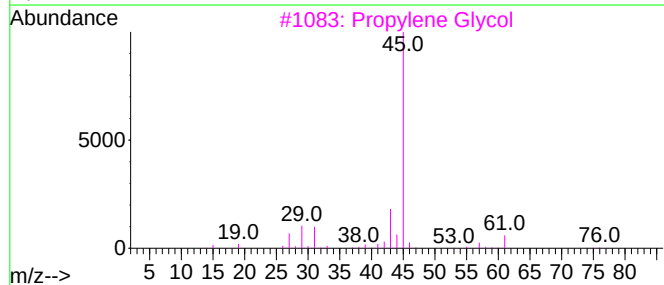
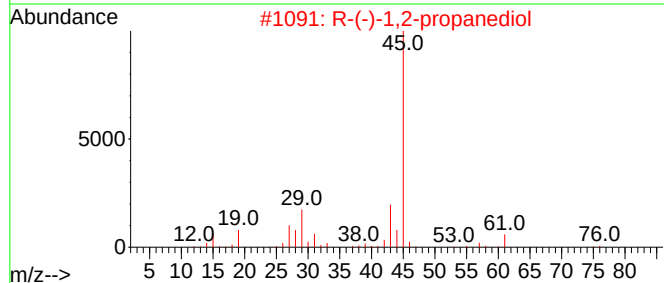
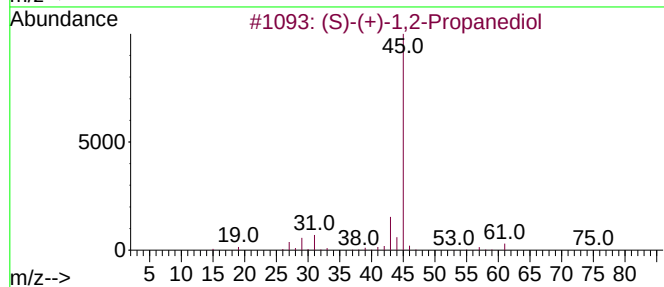
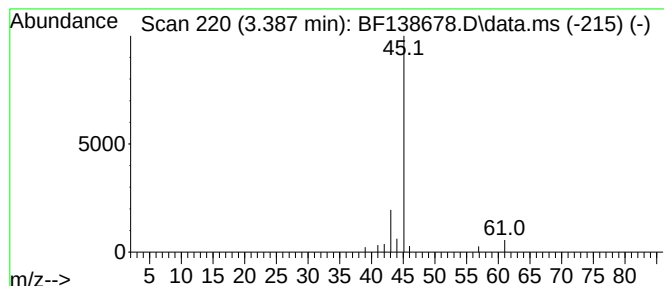
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	2.14 ng	64618	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	64
3	Propylene Glycol			76	C3H8O2	000057-55-6	9
4	Isopropyl Alcohol			60	C3H8O	000067-63-0	9
5	Formamide			45	CH3NO	000075-12-7	7



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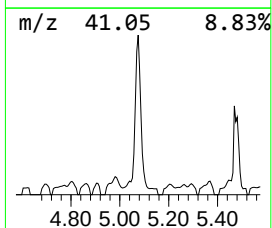
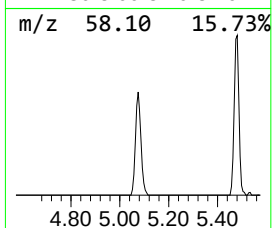
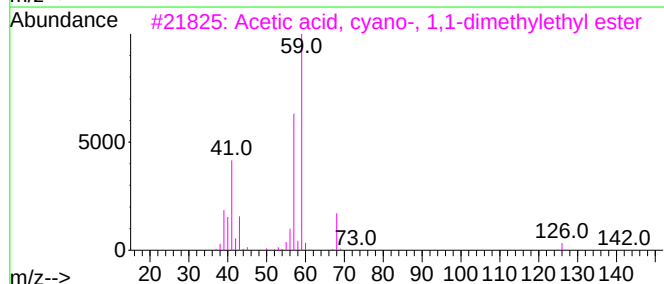
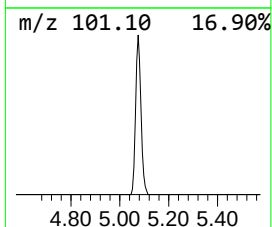
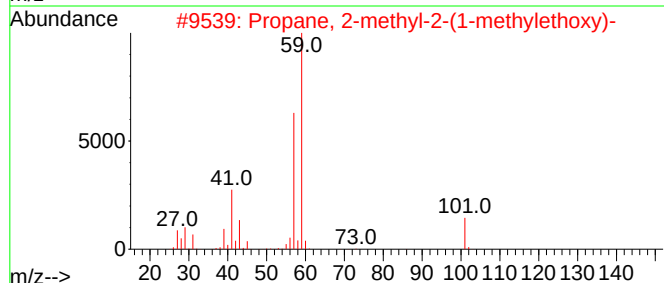
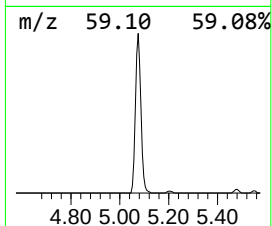
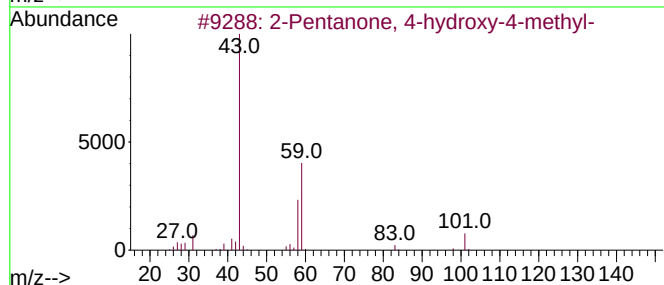
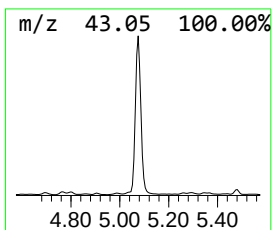
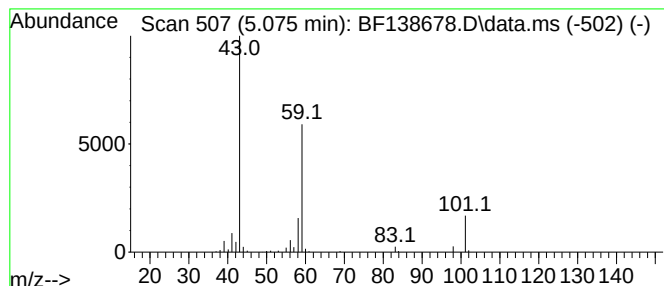
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	5.37 ng	162360	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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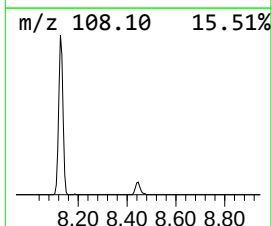
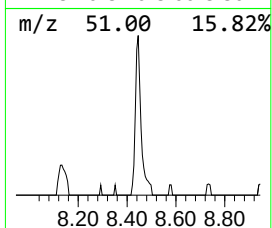
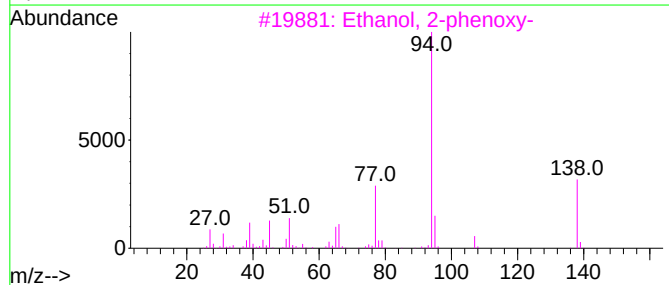
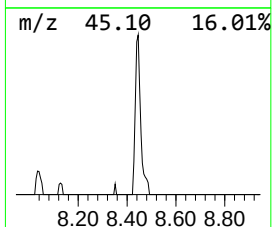
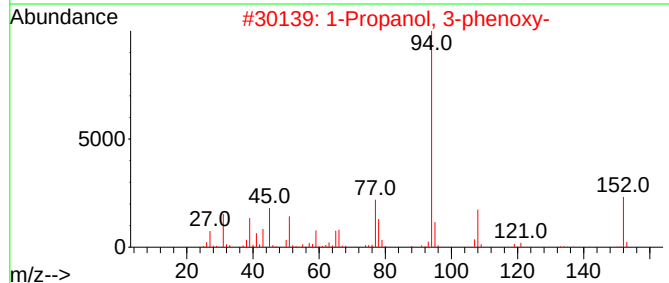
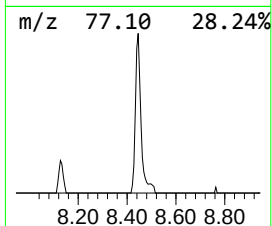
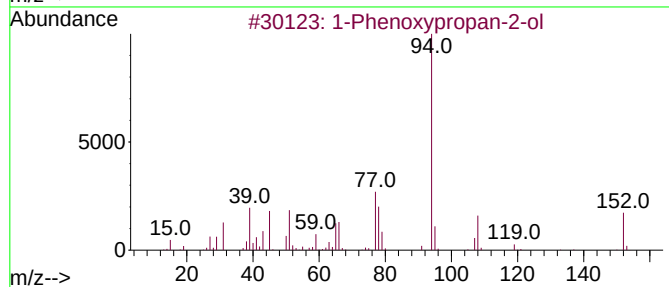
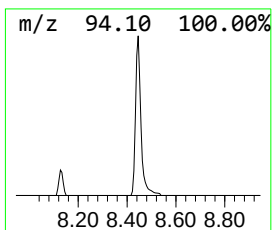
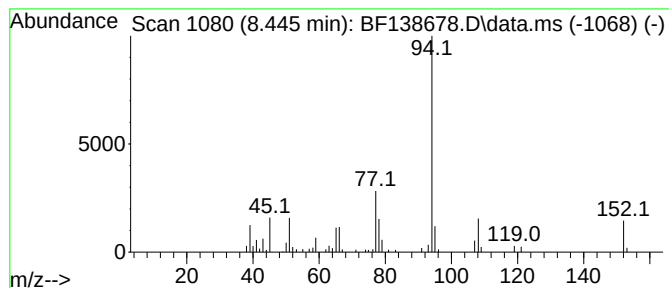
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	2.29 ng	82829	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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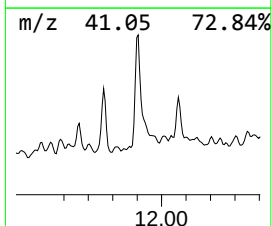
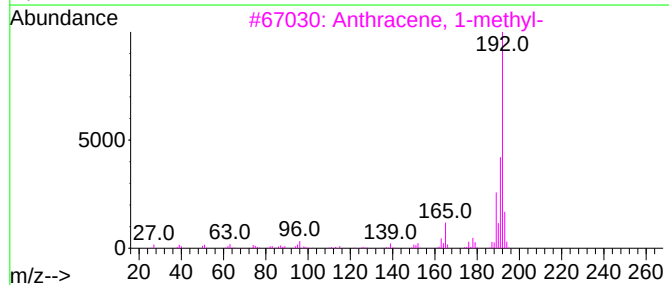
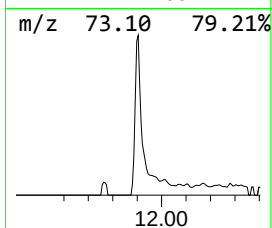
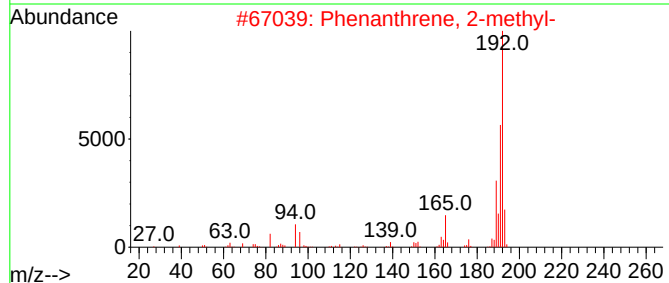
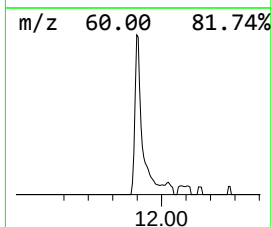
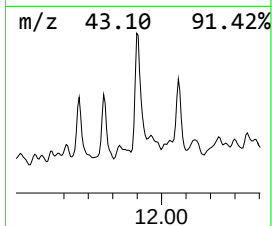
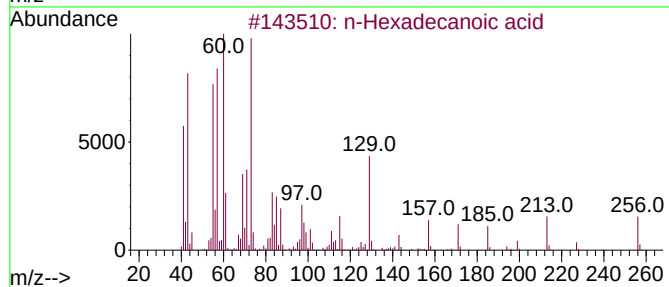
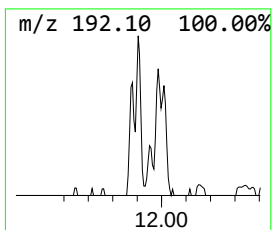
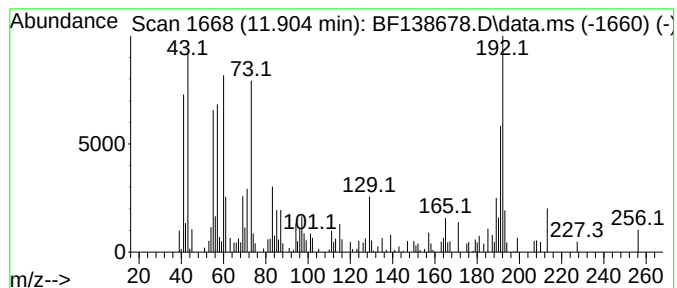
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	3.59 ng	103232	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	80
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	49
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	43



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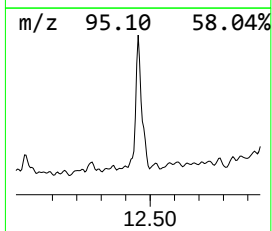
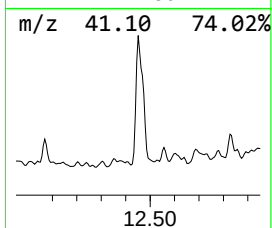
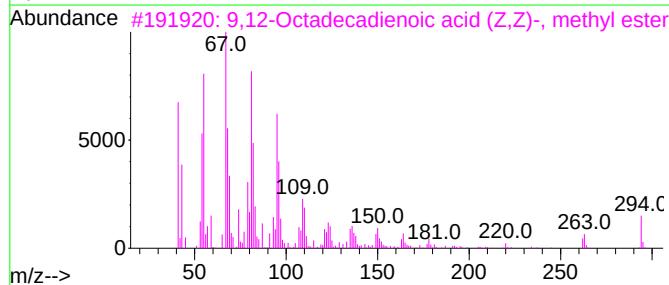
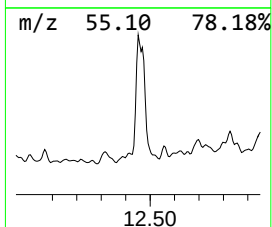
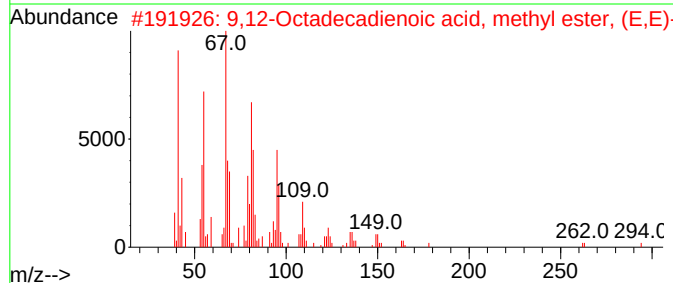
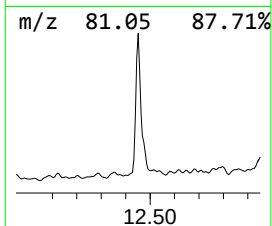
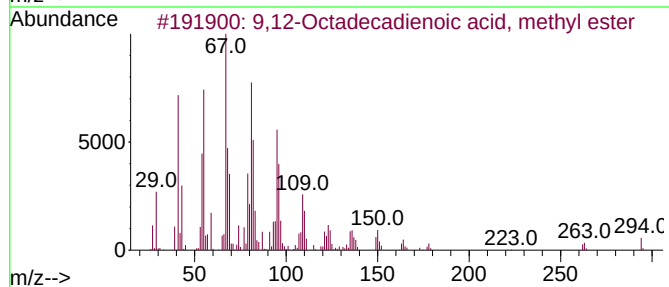
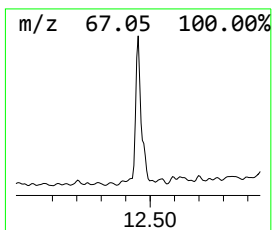
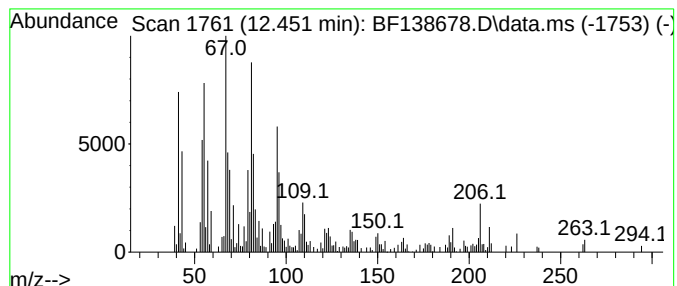
Instrument :
BNA_F
ClientSampleId :
TR-06-07252024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.451	9.29 ng	267147	Phenanthrene-d10	11.374	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	98
5	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072924\
Data File : BF138678.D
Acq On : 29 Jul 2024 19:47
Operator : RC/JU
Sample : P3367-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-07252024

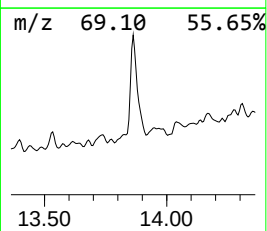
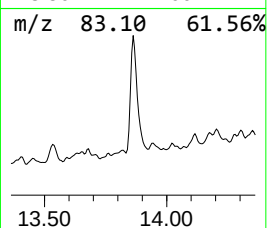
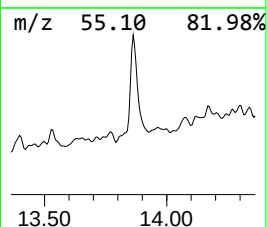
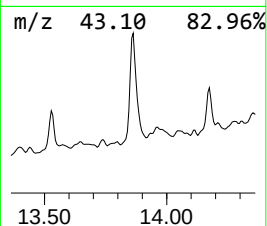
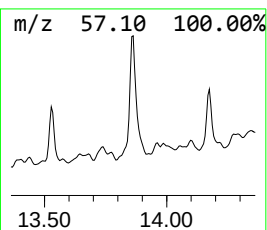
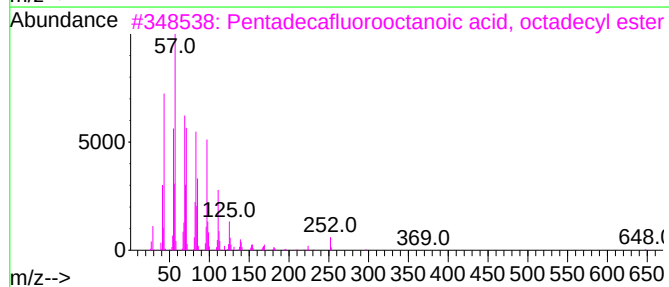
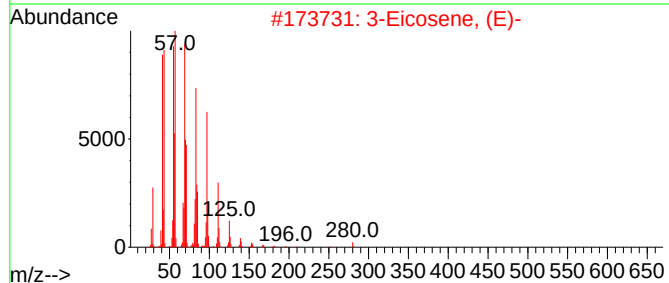
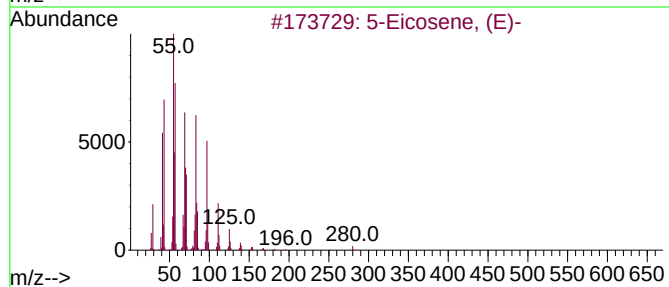
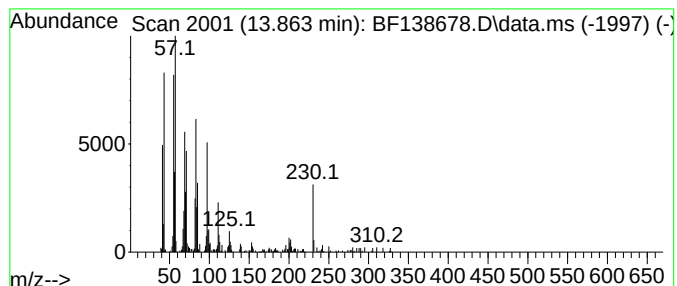
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	6.01 ng	154664	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
4			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	87
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072924\
Data File : BF138678.D
Acq On : 29 Jul 2024 19:47
Operator : RC/JU
Sample : P3367-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-07252024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	86.4	ng	2611210	1	6.845	604702	20.0
(S)-(+)-1,2-Pro...	3.387	2.1	ng	64618	1	6.845	604702	20.0
2-Pentanone, 4-...	5.075	5.4	ng	162360	1	6.845	604702	20.0
1-Phenoxypropan...	8.445	2.3	ng	82829	2	8.128	722812	20.0
n-Hexadecanoic ...	11.904	3.6	ng	103232	4	11.374	575300	20.0
9,12-Octadecadi...	12.451	9.3	ng	267147	4	11.374	575300	20.0
5-Eicosene, (E)-	13.863	6.0	ng	154664	5	14.015	515025	20.0