

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
 Data File : BM047377.D
 Acq On : 28 Aug 2024 12:22
 Operator : RC/JU
 Sample : P3739-09
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-2

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_M\Methods\8270-BM082624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047377.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.252	58	62	78	rBV	468645	622912	4.64%	0.680%
2	4.557	276	284	292	rBV	280741	405435	3.02%	0.442%
3	5.010	354	361	379	rBV	4264259	6220918	46.34%	6.790%
4	6.575	620	627	639	rBV	4212135	6771783	50.44%	7.391%
5	6.981	691	696	713	rBV2	176751	392171	2.92%	0.428%
6	7.345	751	758	768	rBV	938433	1459856	10.87%	1.593%
7	8.498	947	954	975	rVB	2658481	4375133	32.59%	4.775%
8	10.104	1220	1227	1232	rBV	1177259	1976915	14.72%	2.158%
9	10.863	1350	1356	1369	rBV	277060	570460	4.25%	0.623%
10	12.616	1646	1654	1674	rBV	6451236	9746135	72.59%	10.637%
11	14.010	1884	1891	1898	rBV	1946791	2820986	21.01%	3.079%
12	14.251	1925	1932	1933	rBV	3292943	4748695	35.37%	5.183%
13	14.269	1933	1935	1950	rVB	4300108	4833031	36.00%	5.275%
14	15.527	2141	2149	2158	rBV	6021355	8965173	66.78%	9.785%
15	16.774	2356	2361	2366	rBV	2382382	3478020	25.91%	3.796%
16	16.815	2366	2368	2375	rVB	487370	640331	4.77%	0.699%
17	16.910	2380	2384	2391	rVB	200491	297489	2.22%	0.325%
18	17.198	2429	2433	2439	rBV	95688	137182	1.02%	0.150%
19	17.480	2477	2481	2491	rVB	103792	168407	1.25%	0.184%
20	17.715	2515	2521	2528	rBV2	1683685	2474097	18.43%	2.700%
21	17.845	2539	2543	2548	rBV	83766	137733	1.03%	0.150%
22	18.257	2609	2613	2622	rVB2	136965	226813	1.69%	0.248%
23	18.592	2665	2670	2675	rBV3	68413	146057	1.09%	0.159%
24	18.856	2710	2715	2720	rBV	1109009	1514500	11.28%	1.653%
25	19.015	2737	2742	2754	rBV	784656	1370838	10.21%	1.496%
26	19.198	2768	2773	2774	rBV2	365508	477653	3.56%	0.521%
27	19.221	2774	2777	2784	rVB	900438	1231975	9.18%	1.345%
28	19.445	2810	2815	2820	rVB	10639032	13425832	100.00%	14.653%
29	20.151	2932	2935	2940	rBV3	115491	157033	1.17%	0.171%
30	20.286	2955	2958	2962	rVB2	118555	141390	1.05%	0.154%
31	20.492	2990	2993	2999	rBV	121443	152220	1.13%	0.166%
32	20.750	3033	3037	3042	rVB	796867	942049	7.02%	1.028%
33	20.956	3069	3072	3075	rBV	167059	196183	1.46%	0.214%
34	21.021	3076	3083	3087	rVV2	2708228	4619206	34.41%	5.041%
35	21.062	3087	3090	3101	rVB	764782	1094081	8.15%	1.194%
36	21.227	3115	3118	3125	rVB	165946	202830	1.51%	0.221%

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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_M\Methods\8270-BM082624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.880	3394	3399	3404	rBV	418056	898091	6.69%	0.980%
38	23.721	3535	3542	3566	rVB	1419271	3585917	26.71%	3.914%

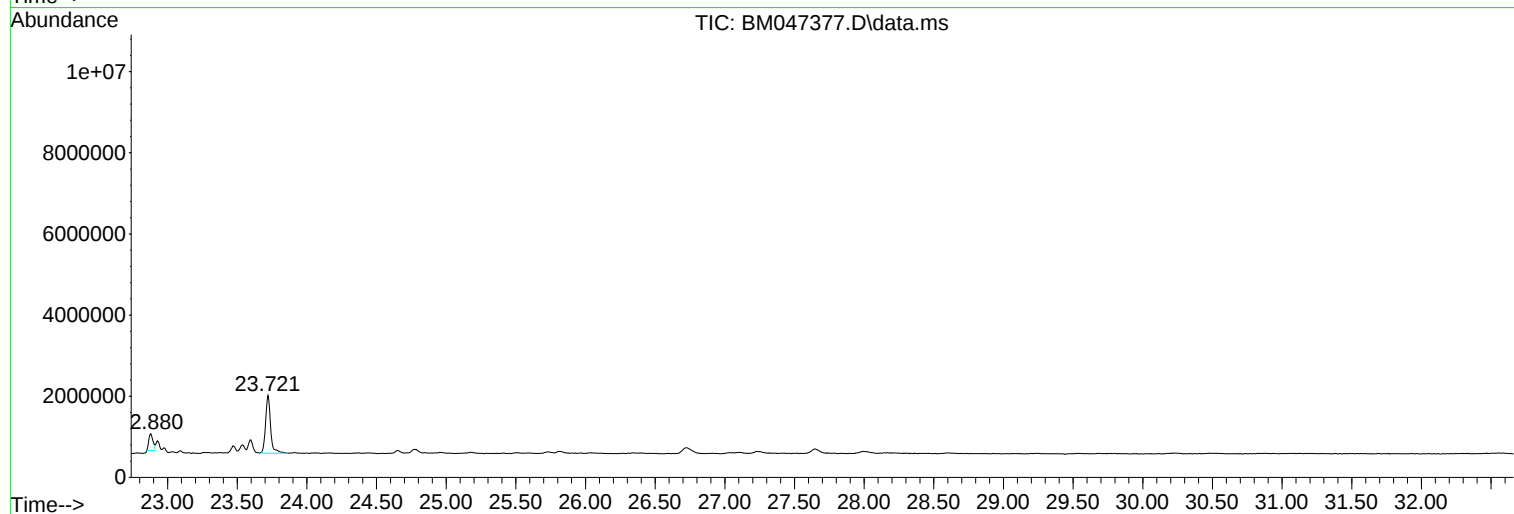
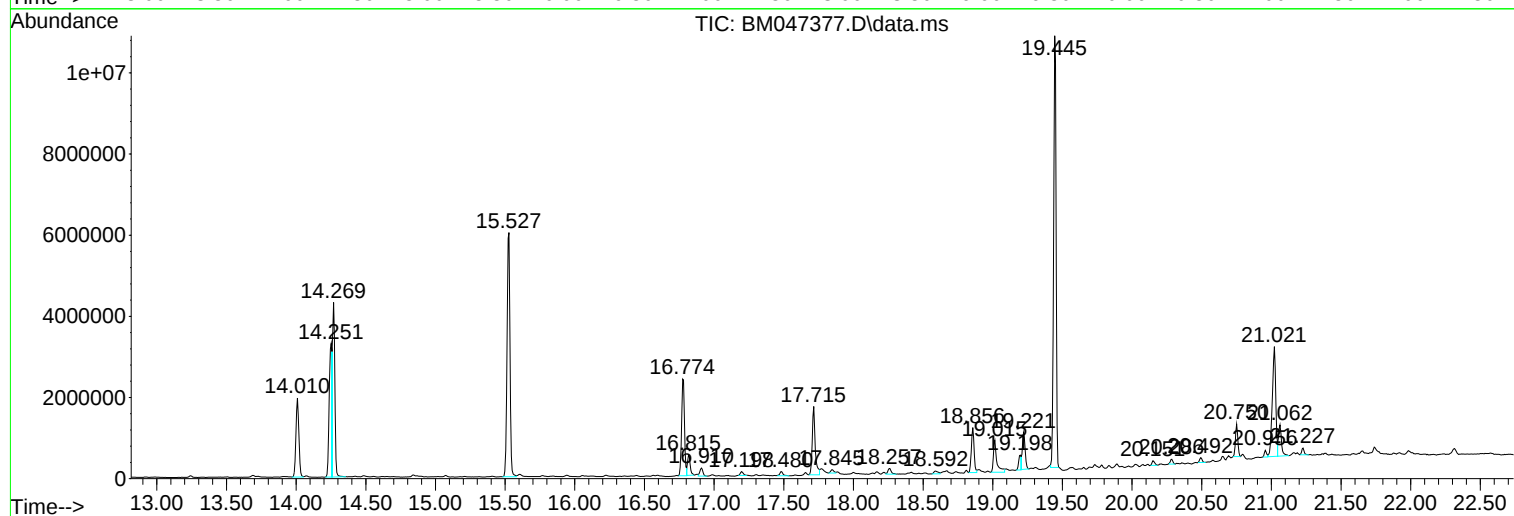
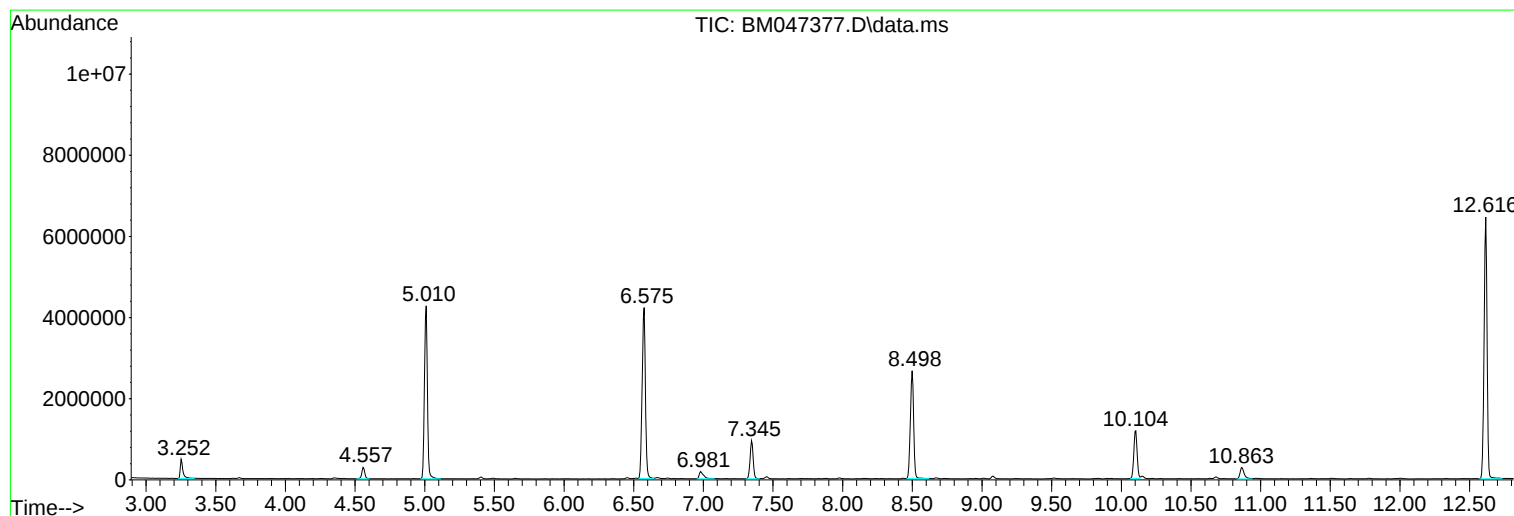
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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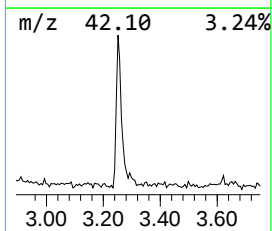
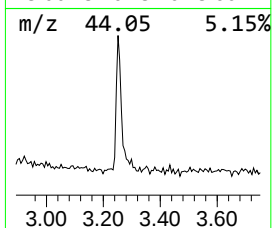
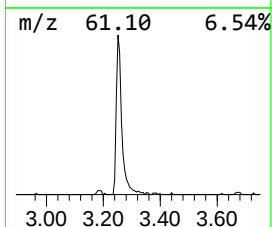
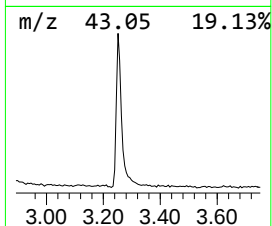
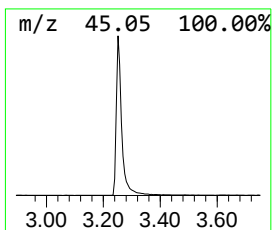
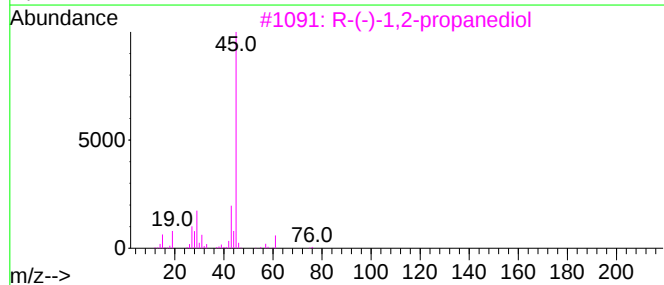
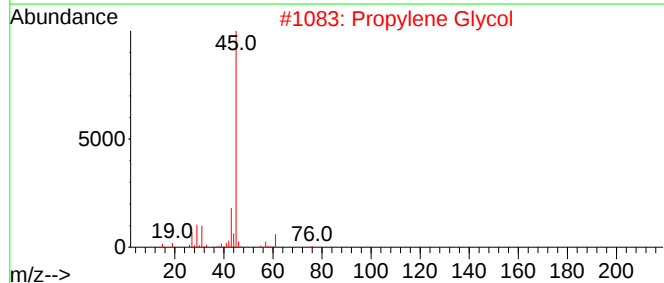
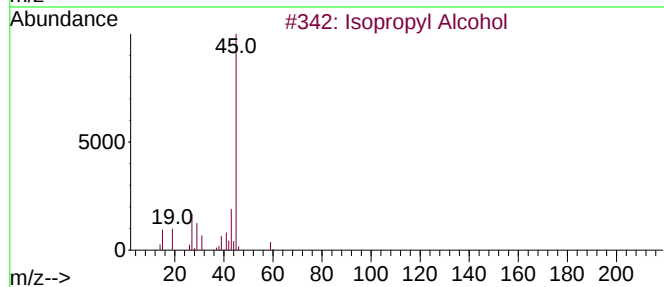
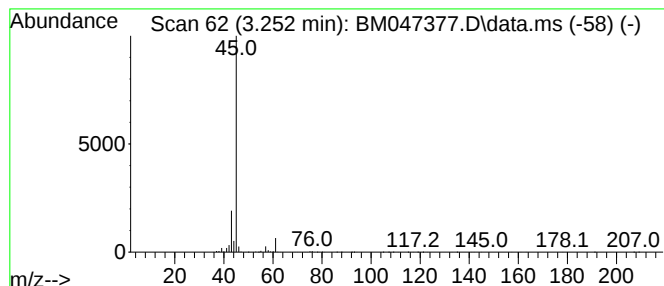
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.252	8.53 ng	622912	1,4-Dichlorobenzene-d4	7.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2			Propylene Glycol	76	C3H8O2	000057-55-6	43
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5			Formamide	45	CH3NO	000075-12-7	7



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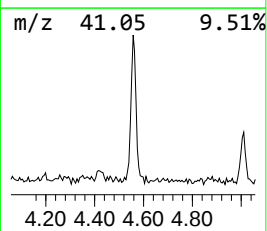
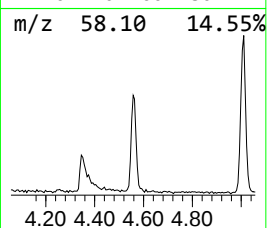
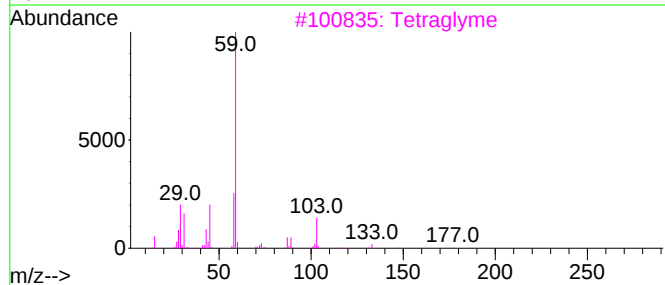
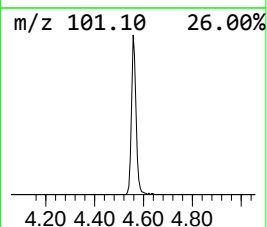
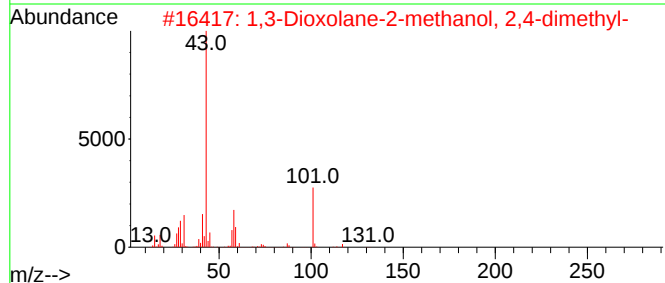
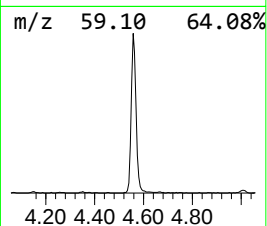
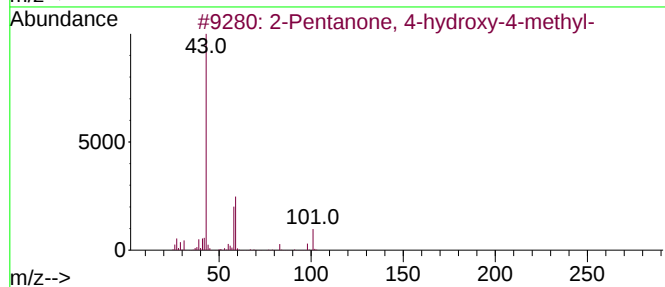
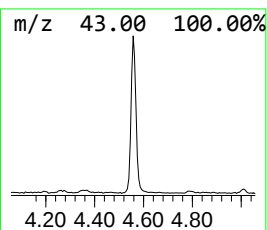
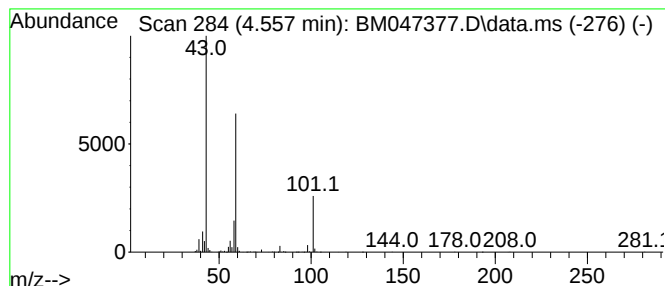
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.557	5.55 ng	405435	1,4-Dichlorobenzene-d4			7.345
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	72
2	1,3-Dioxolane-2-methanol, 2,4-di...		132	C6H12O3	053951-43-2	28
3	Tetraglyme		222	C10H22O5	000143-24-8	25
4	5-Hexen-2-one		98	C6H10O	000109-49-9	9
5	(+) -4-Amino-4,5-dihydro-2(3H)-f...		101	C4H7NO2	016504-58-8	9



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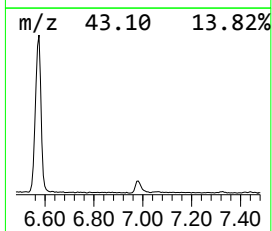
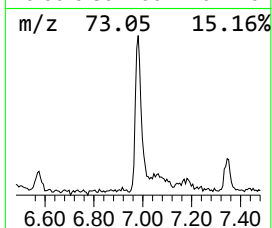
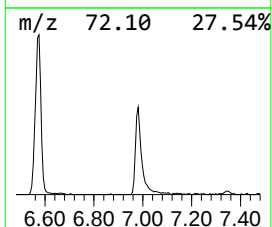
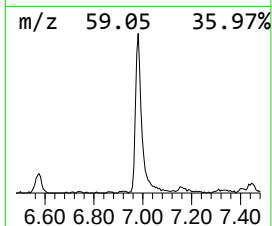
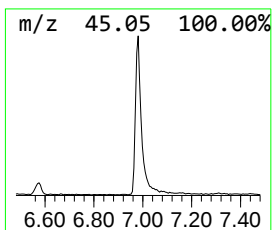
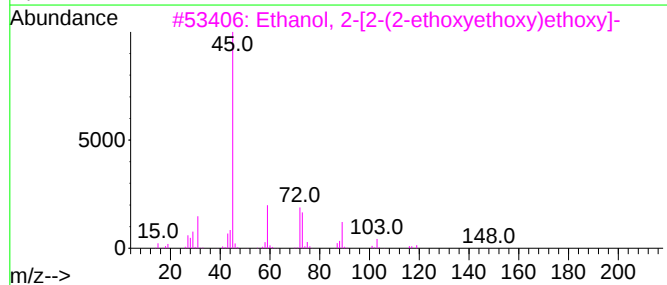
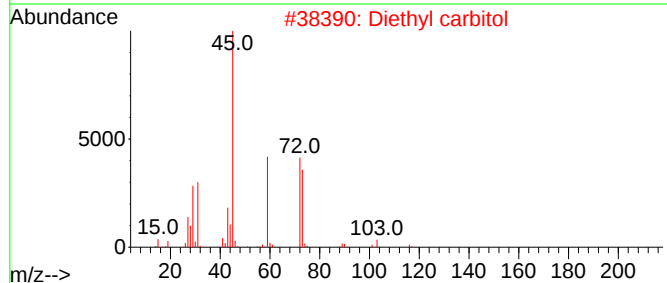
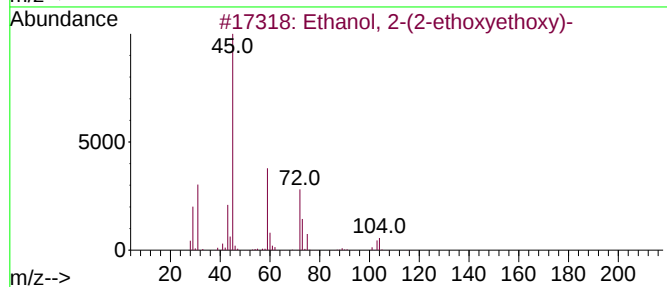
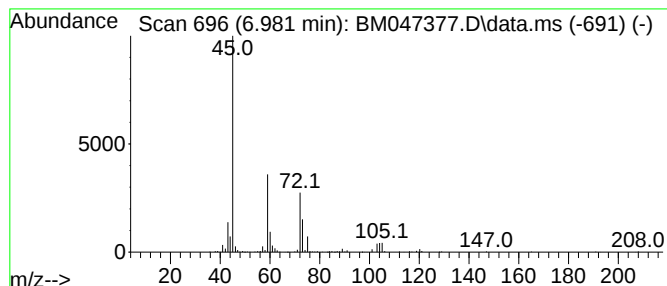
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	5.37 ng	392171	1,4-Dichlorobenzene-d4	7.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	43



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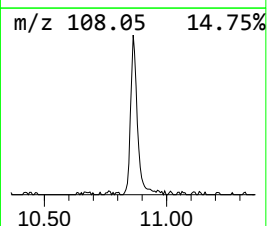
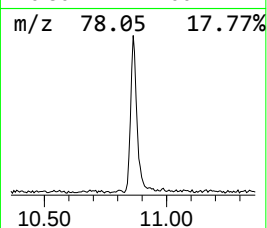
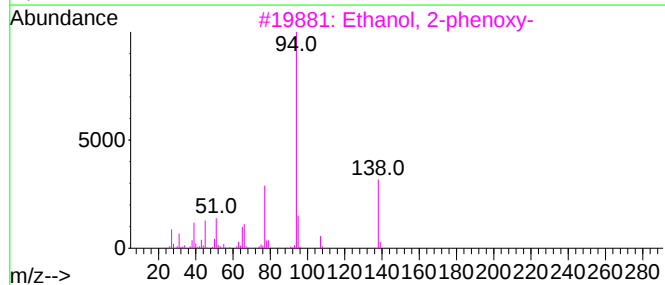
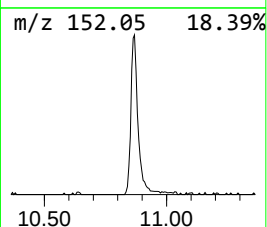
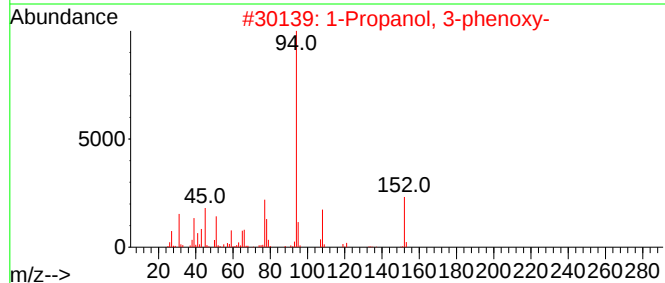
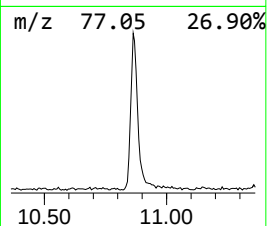
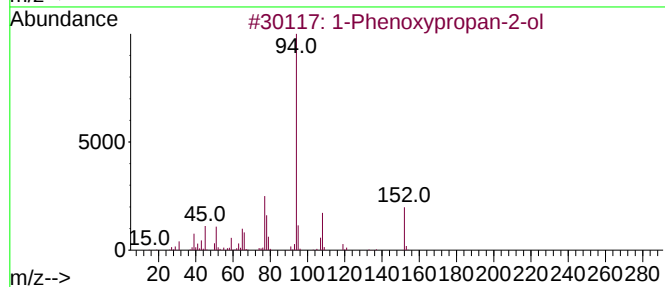
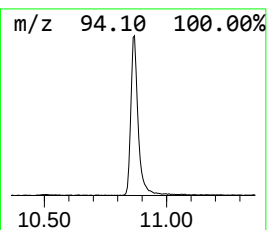
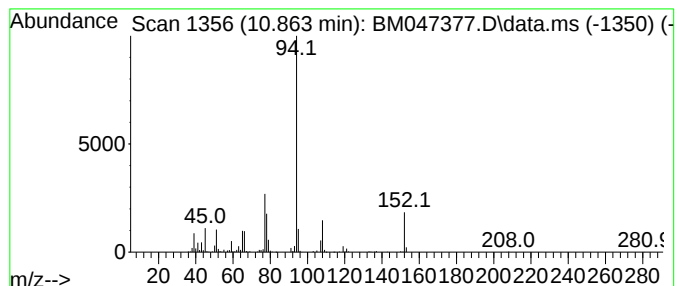
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.863	5.77 ng	570460	Naphthalene-d8	10.104

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	83
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5			Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	53



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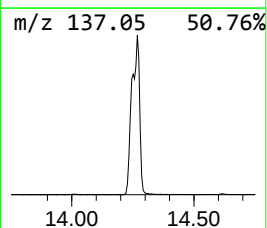
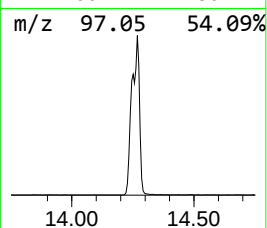
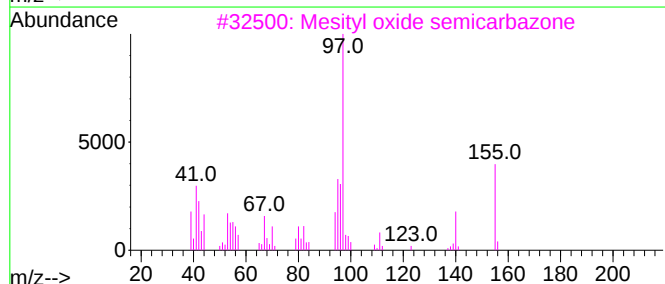
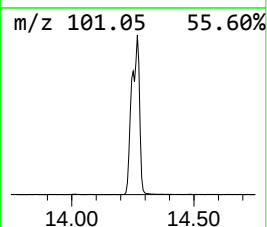
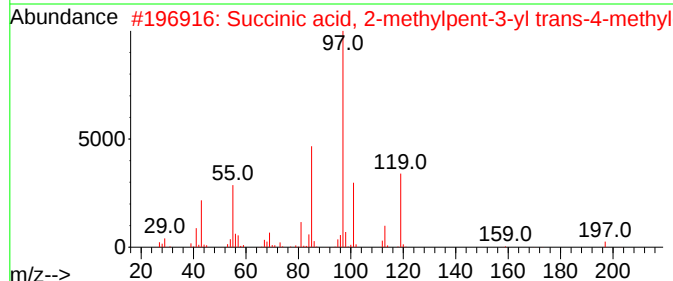
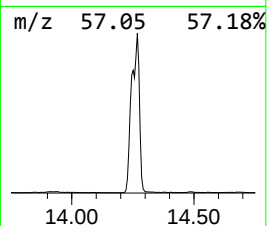
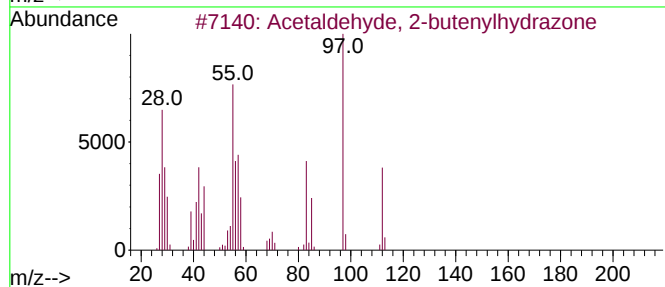
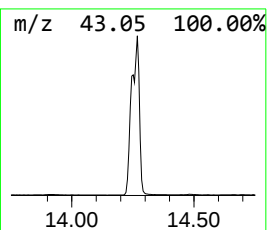
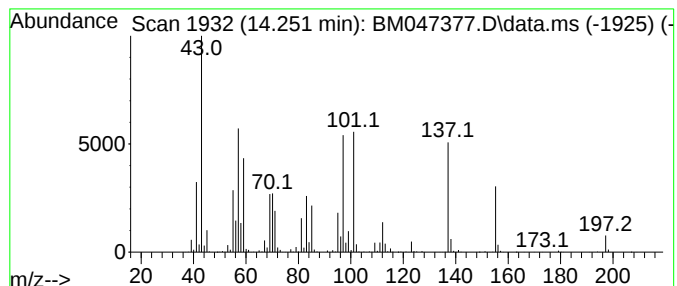
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.251 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.251	33.67 ng	4748700	Acenaphthene-d10	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde, 2-butenylhydrazone	112	C6H12N2	075268-07-4	14
2			Succinic acid, 2-methylpent-3-yl...	298	C17H30O4	1000390-06-8	14
3			Mesityl oxide semicarbazone	155	C7H13N3O	003780-62-9	14
4			2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	14
5			Thiophene, 3-ethyl-	112	C6H8S	001795-01-3	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
Data File : BM047377.D
Acq On : 28 Aug 2024 12:22
Operator : RC/JU
Sample : P3739-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-2

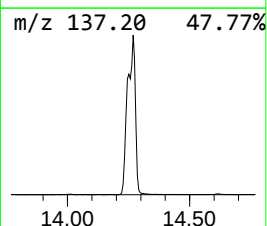
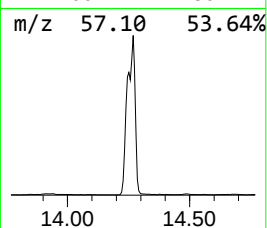
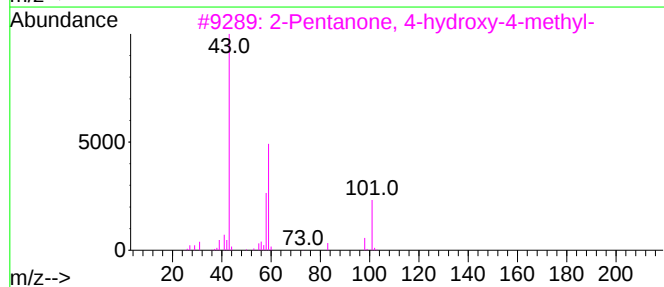
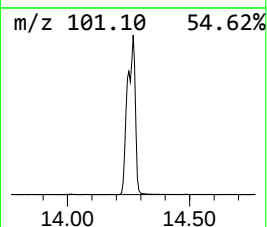
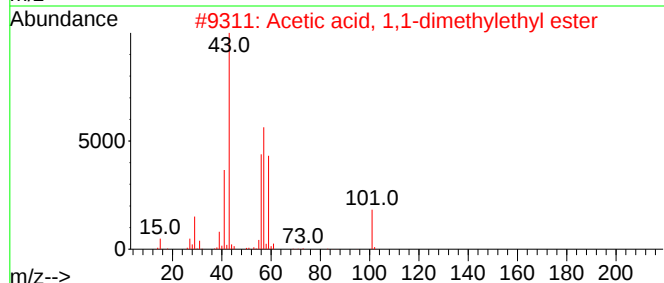
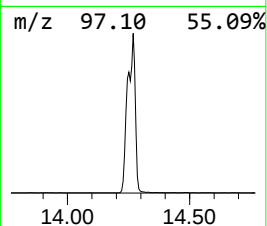
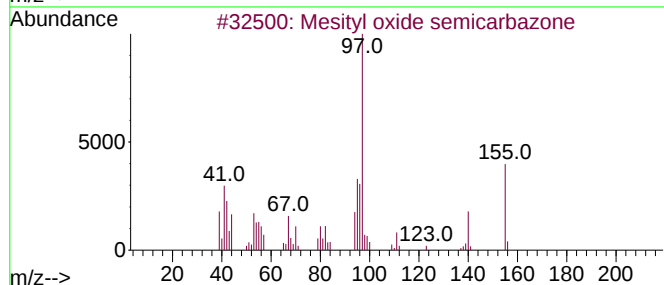
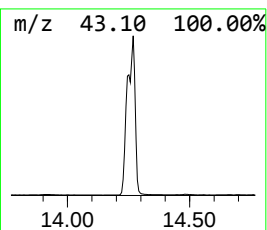
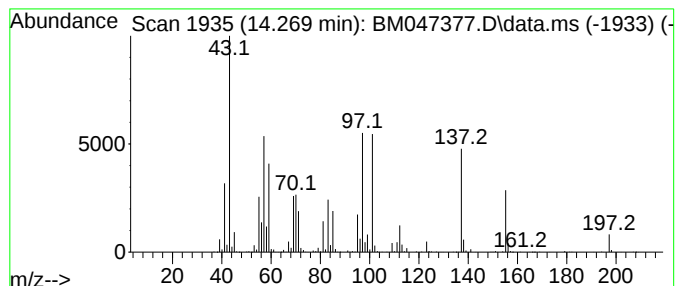
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.269 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	34.26 ng	4833030	Acenaphthene-d10	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesityl oxide semicarbazone	155	C7H13N3O	003780-62-9	18
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	12
3			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	12
4			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	11
5			Succinic acid, butyl 3,3-dimethy...	258	C14H26O4	1000349-50-8	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
Data File : BM047377.D
Acq On : 28 Aug 2024 12:22
Operator : RC/JU
Sample : P3739-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-2

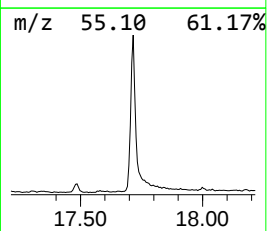
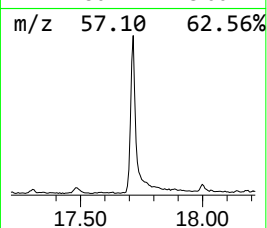
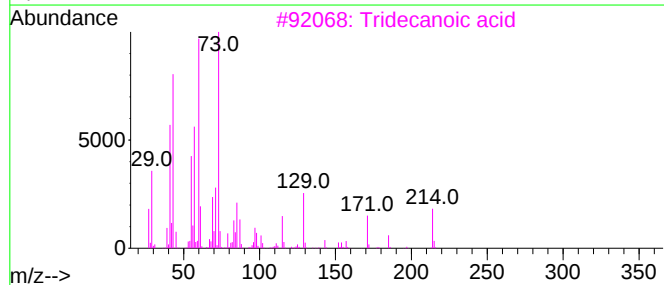
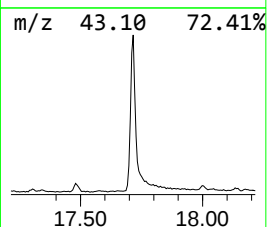
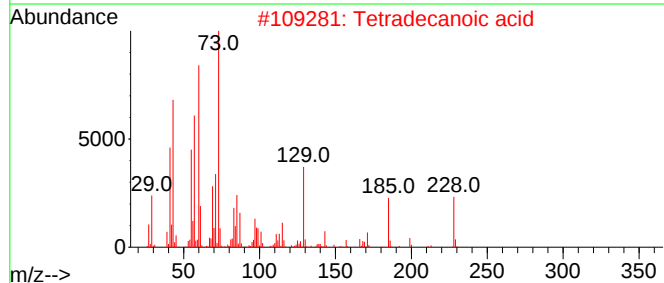
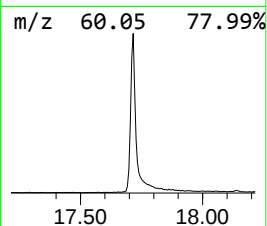
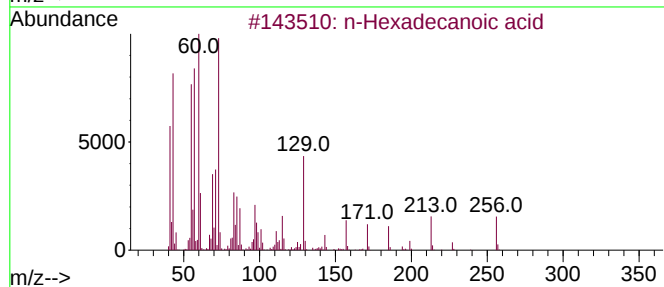
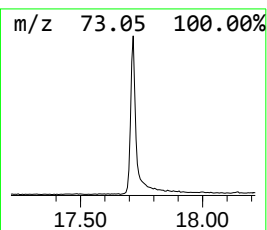
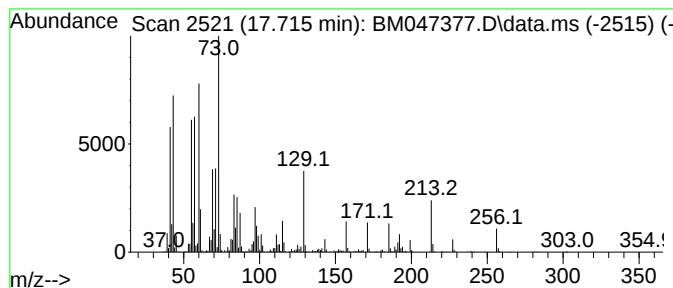
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	14.23 ng	2474100	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
Data File : BM047377.D
Acq On : 28 Aug 2024 12:22
Operator : RC/JU
Sample : P3739-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-2

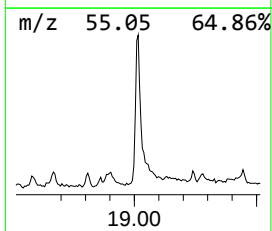
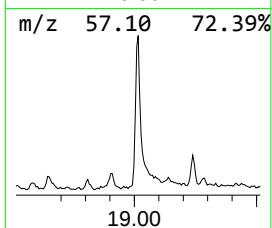
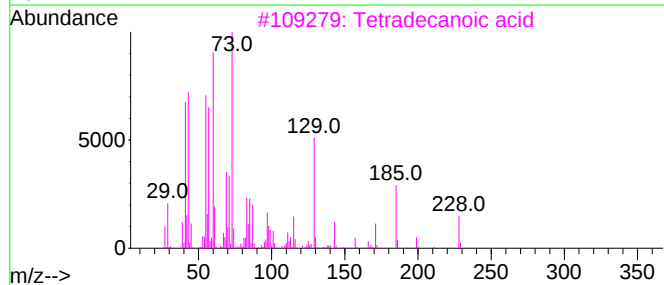
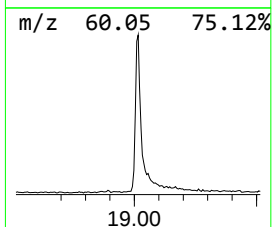
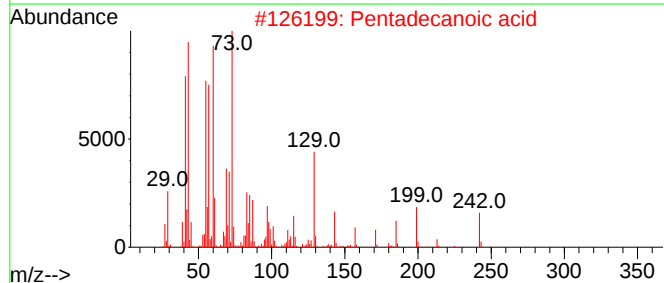
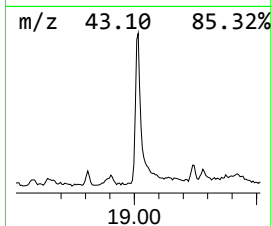
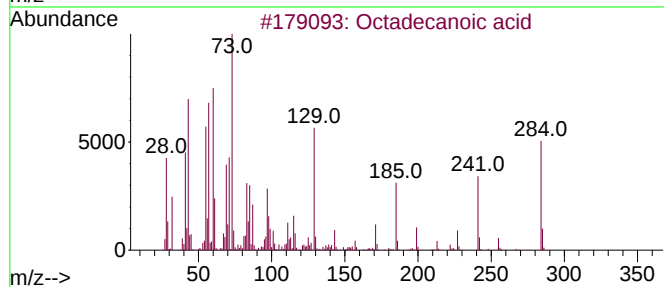
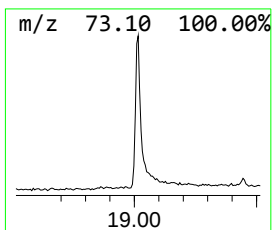
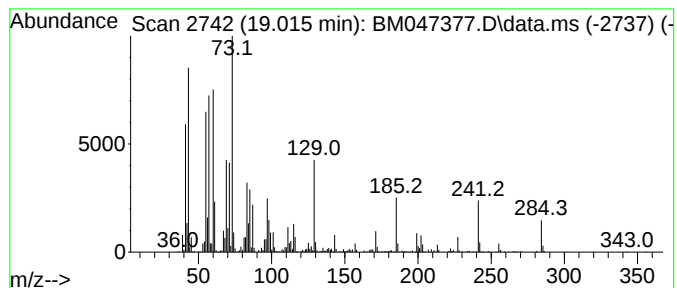
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	5.94 ng	1370840	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
Data File : BM047377.D
Acq On : 28 Aug 2024 12:22
Operator : RC/JU
Sample : P3739-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

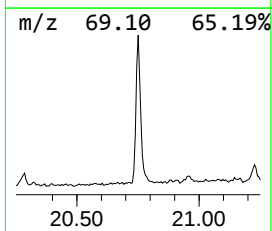
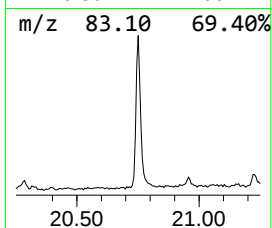
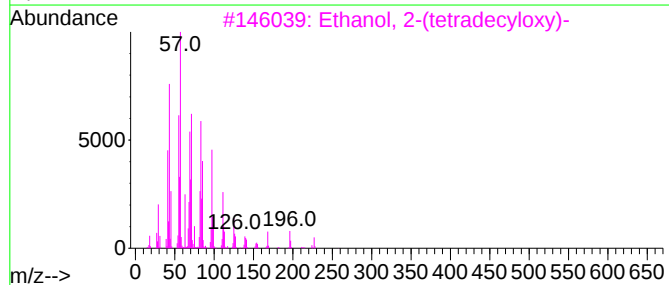
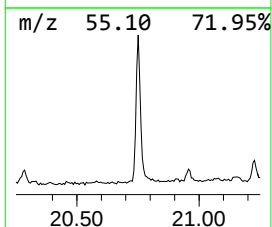
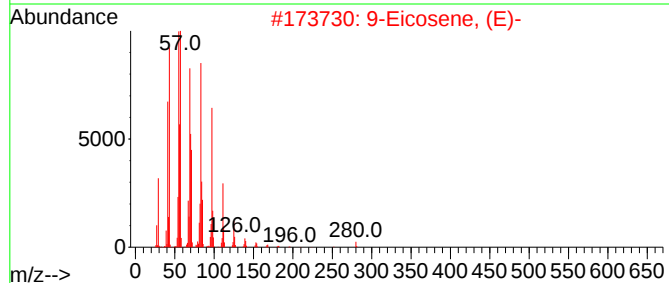
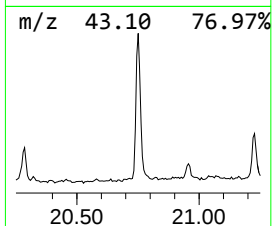
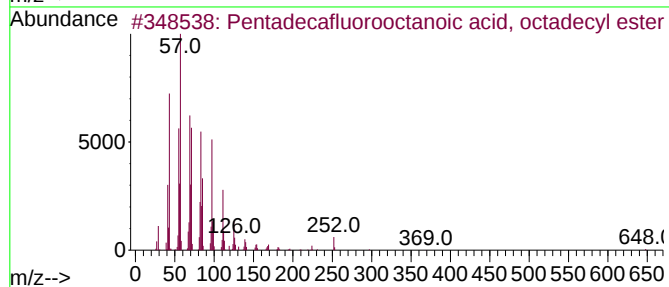
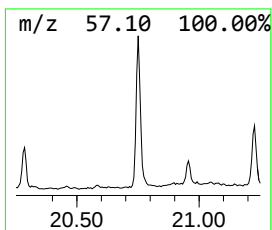
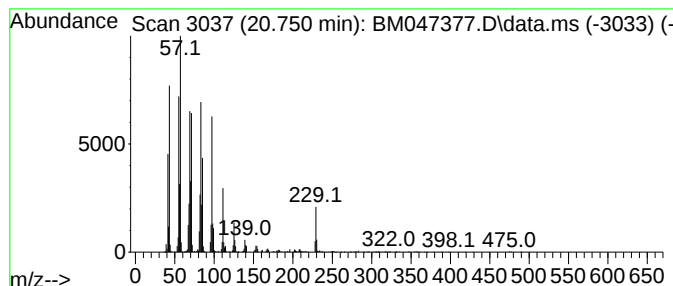
Instrument :
BNA_M
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecafluorooctanoic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.750	4.08 ng	942049	Chrysene-d12	21.021	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
Data File : BM047377.D
Acq On : 28 Aug 2024 12:22
Operator : RC/JU
Sample : P3739-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	3.252	8.5	ng	622912	1	7.345	1459860	20.0
2-Pentanone, 4-...	4.557	5.5	ng	405435	1	7.345	1459860	20.0
Ethanol, 2-(2-e...	6.981	5.4	ng	392171	1	7.345	1459860	20.0
1-Phenoxypropan...	10.863	5.8	ng	570460	2	10.104	1976920	20.0
unknown14.251	14.251	33.7	ng	4748700	3	14.010	2820990	20.0
unknown14.269	14.269	34.3	ng	4833030	3	14.010	2820990	20.0
n-Hexadecanoic ...	17.715	14.2	ng	2474100	4	16.774	3478020	20.0
Octadecanoic acid	19.015	5.9	ng	1370840	5	21.021	4619210	20.0
Pentadecafluoro...	20.750	4.1	ng	942049	5	21.021	4619210	20.0