

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
 Data File : BM047384.D
 Acq On : 28 Aug 2024 17:05
 Operator : RC/JU
 Sample : P3767-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P-1-COMPOSITE

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: BM047384.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.257	59	63	70	rBV	129204	188580	1.89%	0.278%
2	4.557	277	284	295	rBV	239903	347518	3.49%	0.513%
3	5.010	354	361	377	rBV	3587255	5249350	52.69%	7.748%
4	6.522	612	618	621	rBV	69114	116023	1.16%	0.171%
5	6.575	621	627	641	rVB	3476287	5591963	56.13%	8.253%
6	6.987	693	697	708	rBV	53380	107896	1.08%	0.159%
7	7.345	748	758	768	rBV	1126992	1785335	17.92%	2.635%
8	8.498	946	954	969	rBV	2335254	3886336	39.01%	5.736%
9	9.081	1048	1053	1060	rBV	62840	114278	1.15%	0.169%
10	10.104	1219	1227	1243	rBV	1445546	2459915	24.69%	3.631%
11	10.869	1349	1357	1368	rBV	201239	421854	4.23%	0.623%
12	11.910	1528	1534	1546	rBV5	54649	149339	1.50%	0.220%
13	12.616	1646	1654	1675	rBV	5984160	9212628	92.47%	13.597%
14	14.010	1884	1891	1900	rBV	2285065	3370028	33.82%	4.974%
15	14.245	1924	1931	1932	rBV3	156605	220043	2.21%	0.325%
16	14.263	1932	1934	1940	rVB2	170563	218700	2.20%	0.323%
17	15.527	2141	2149	2159	rBV	4623040	7209560	72.36%	10.641%
18	16.774	2356	2361	2366	rBV	2566489	3657896	36.71%	5.399%
19	16.821	2366	2369	2373	rVB	197589	249557	2.50%	0.368%
20	16.909	2380	2384	2392	rVB	78827	134146	1.35%	0.198%
21	17.198	2425	2433	2440	rBV2	67160	146211	1.47%	0.216%
22	17.280	2443	2447	2450	rBV2	93677	118435	1.19%	0.175%
23	17.651	2506	2510	2515	rBV2	111735	194851	1.96%	0.288%
24	17.715	2516	2521	2529	rVV2	1060227	1558662	15.64%	2.300%
25	18.209	2601	2605	2610	rVB2	71436	106115	1.07%	0.157%
26	18.856	2710	2715	2719	rBV	595828	838879	8.42%	1.238%
27	19.015	2738	2742	2749	rBV	423895	603294	6.06%	0.890%
28	19.227	2770	2778	2783	rBV	457925	774828	7.78%	1.144%
29	19.445	2810	2815	2825	rVB	7944223	9963251	100.00%	14.705%
30	20.097	2923	2926	2930	rVB2	196528	242593	2.43%	0.358%
31	20.715	3029	3031	3033	rBV	127893	128019	1.28%	0.189%
32	20.750	3033	3037	3043	rVB	938732	1186319	11.91%	1.751%
33	20.956	3070	3072	3076	rVB	150439	141294	1.42%	0.209%
34	21.021	3077	3083	3088	rVV2	2102933	3230427	32.42%	4.768%
35	21.062	3088	3090	3100	rVB	352068	487397	4.89%	0.719%
36	23.038	3422	3426	3433	rVB2	330811	633992	6.36%	0.936%

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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
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37	23.721	3536	3542	3552	rVB	1217638	2707969	27.18%	3.997%
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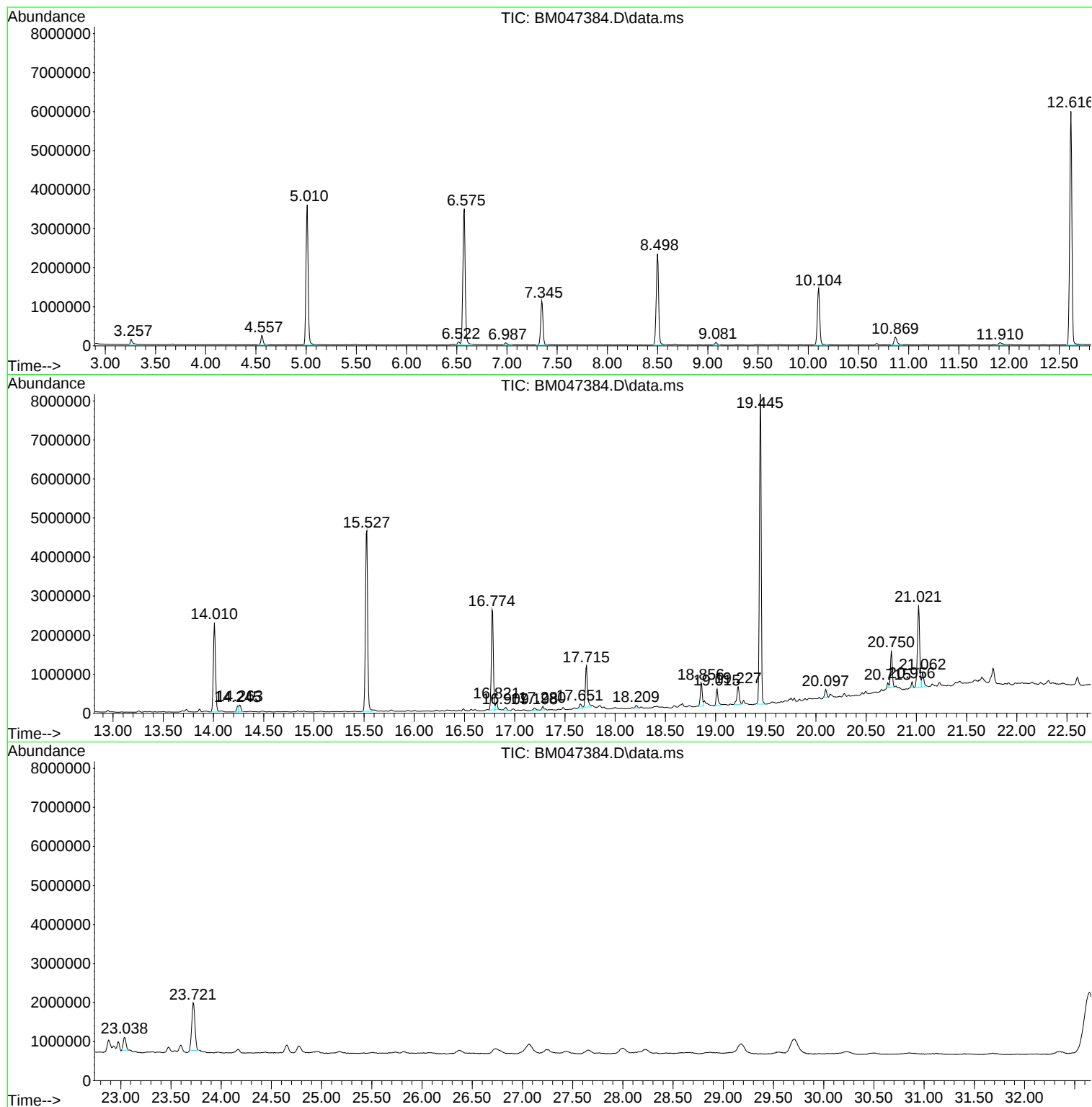
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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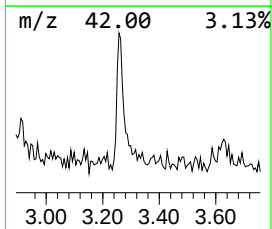
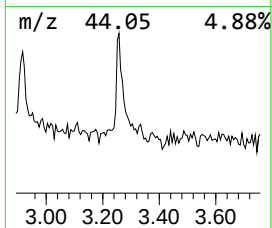
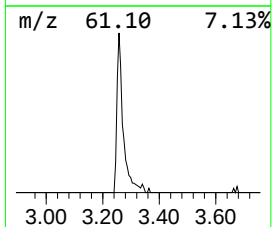
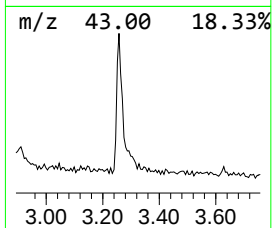
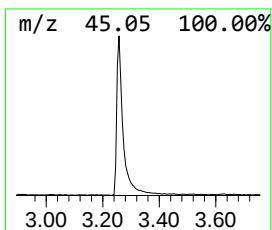
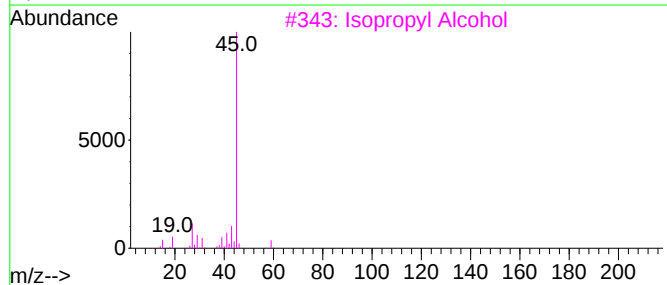
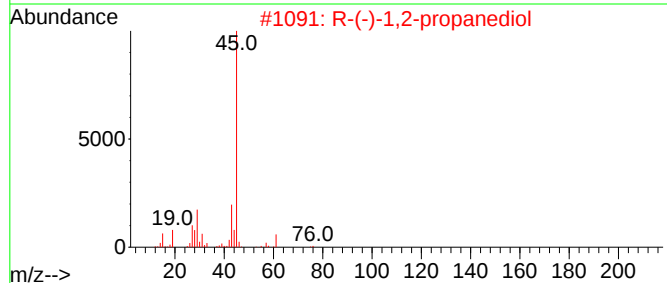
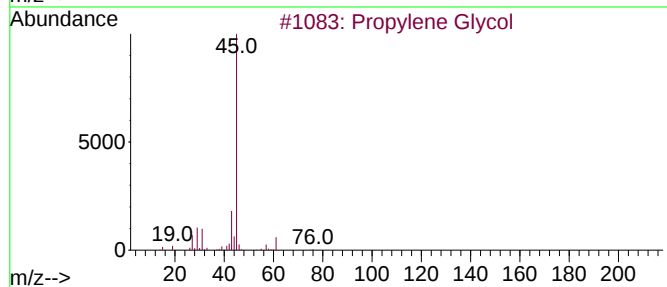
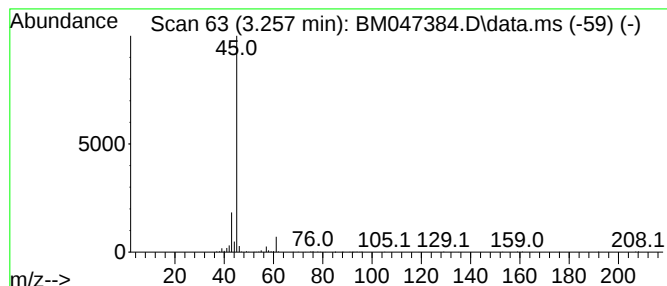
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.257 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.257	2.11 ng	188580	1,4-Dichlorobenzene-d4	7.345

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propylene Glycol	76	C3H8O2	000057-55-6	43
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5		2-Hexanol	102	C6H14O	000626-93-7	9



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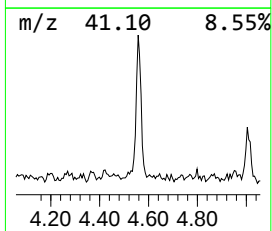
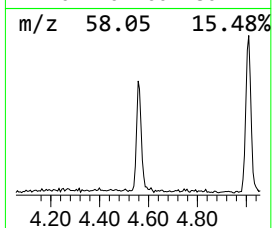
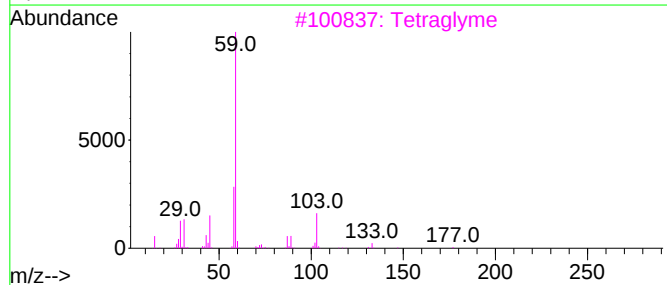
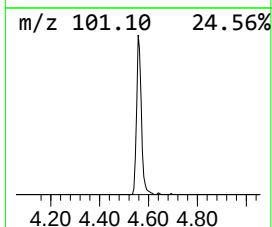
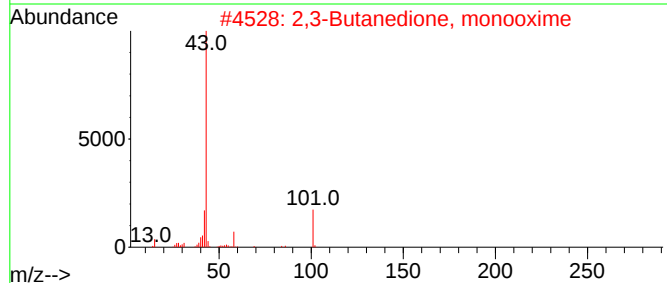
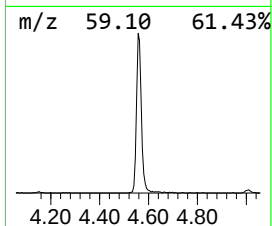
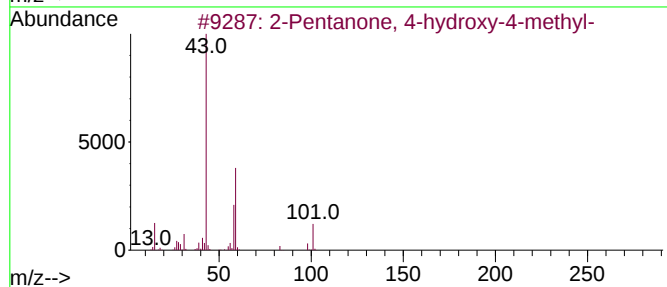
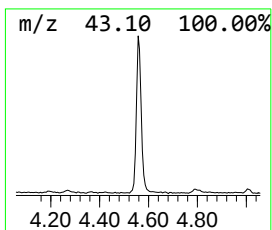
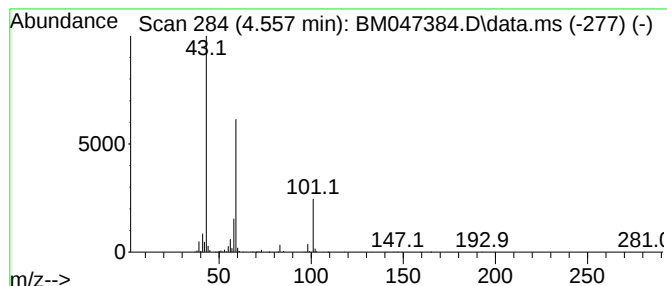
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	3.89 ng	347518	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	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3			Tetraglyme	222	C10H22O5	000143-24-8	32
4			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23



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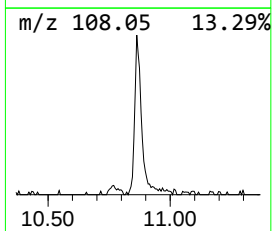
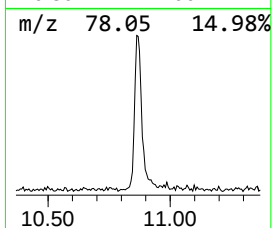
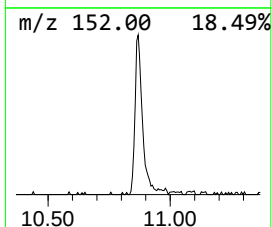
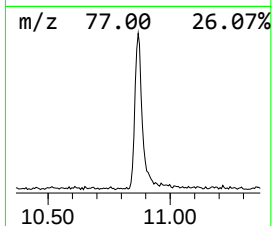
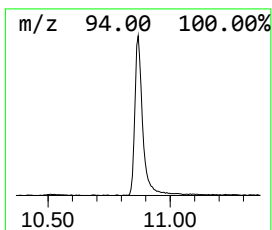
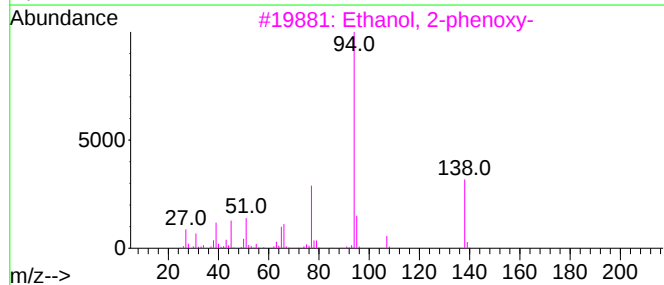
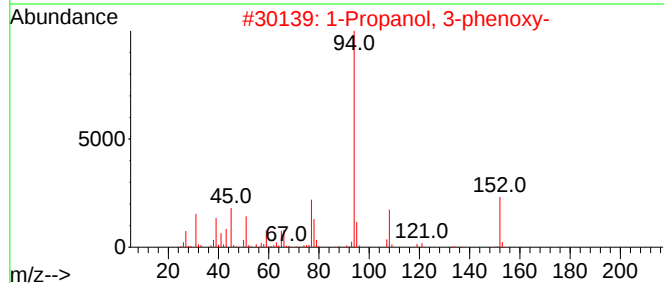
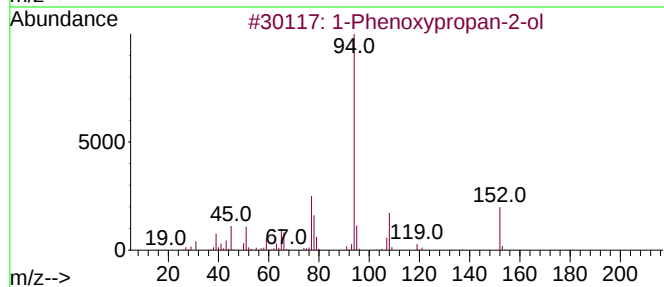
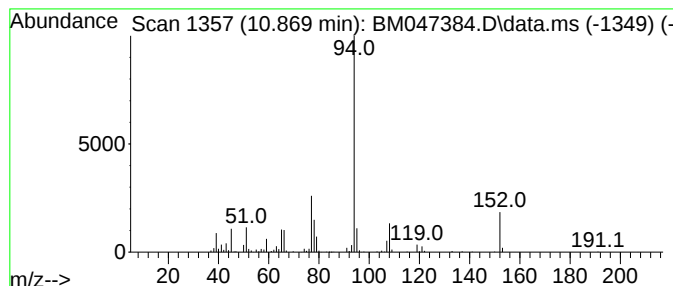
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.869	3.43 ng	421854	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	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	53



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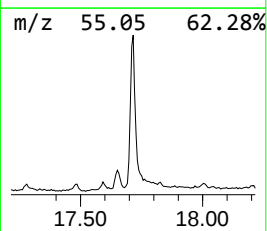
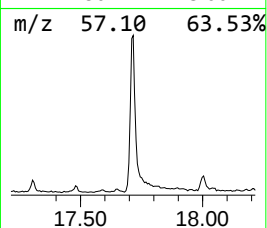
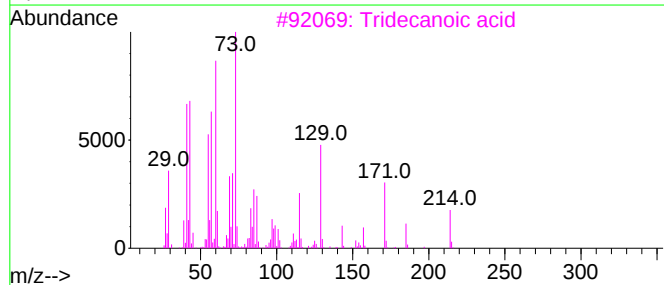
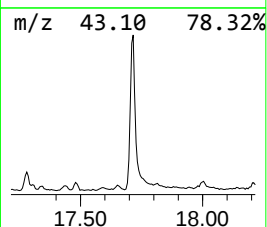
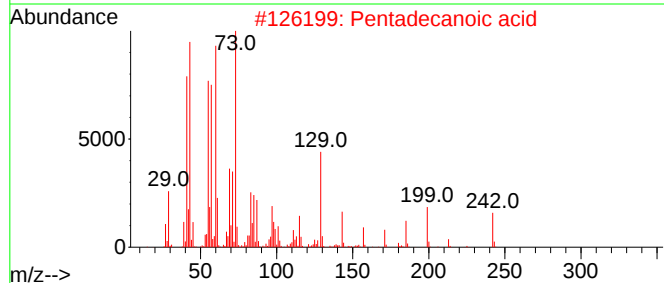
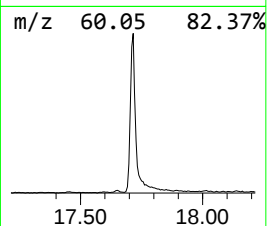
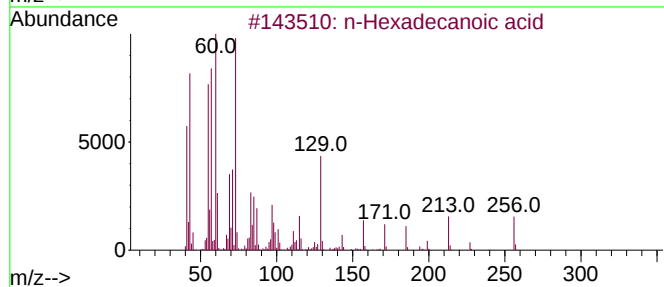
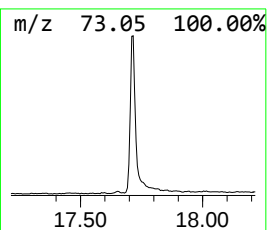
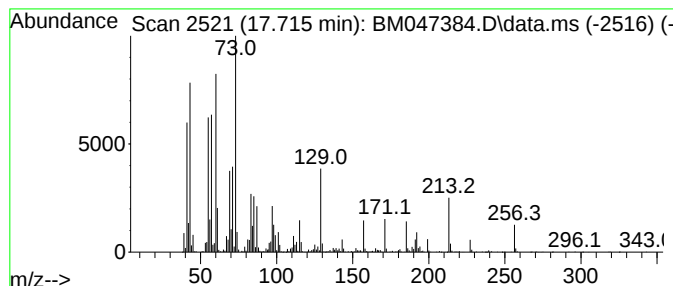
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	8.52 ng	1558660	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5			Octadecanoic acid	284	C18H36O2	000057-11-4	87



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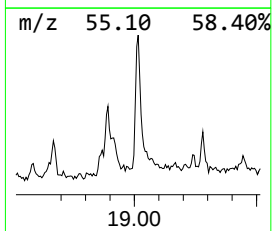
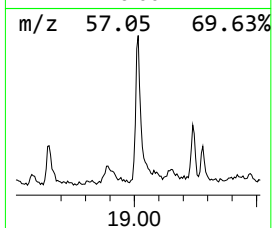
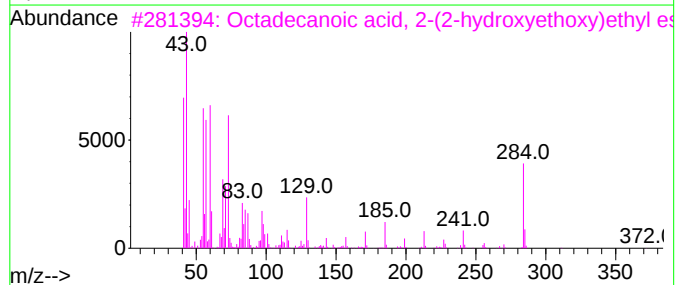
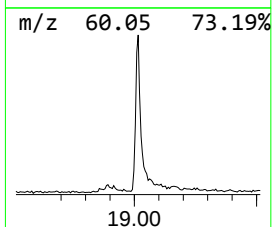
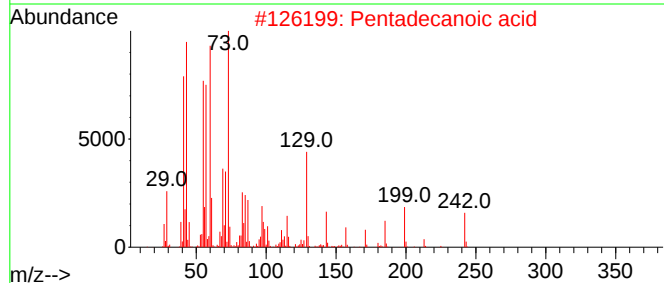
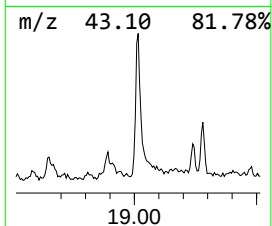
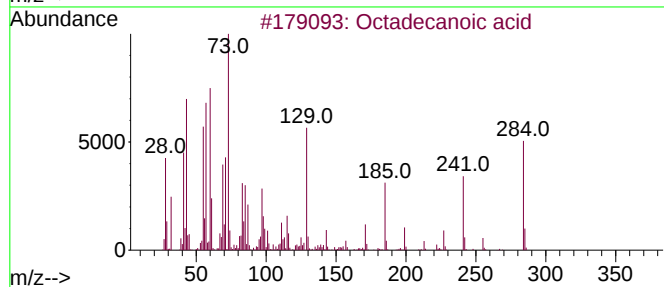
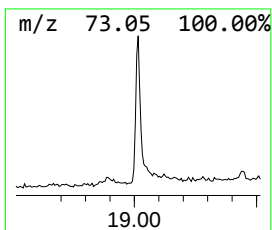
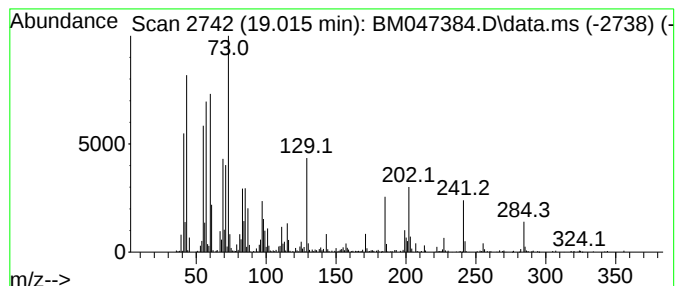
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	3.74 ng	603294	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			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Dodecanoic acid	200	C12H24O2	000143-07-7	70
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
Data File : BM047384.D
Acq On : 28 Aug 2024 17:05
Operator : RC/JU
Sample : P3767-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P-1-COMPOSITE

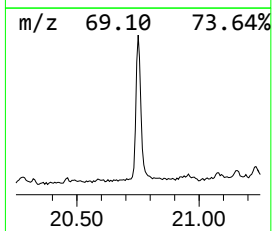
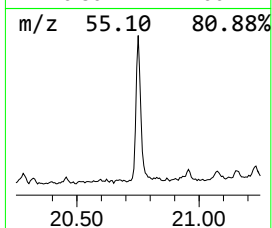
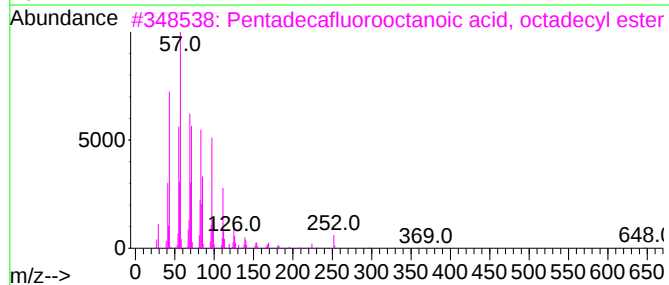
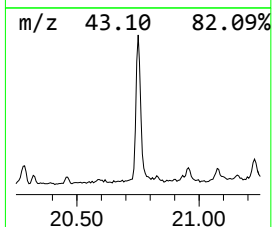
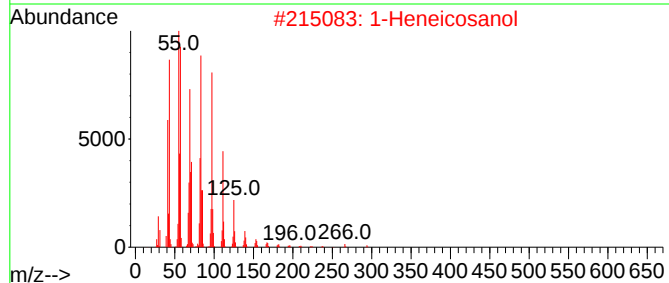
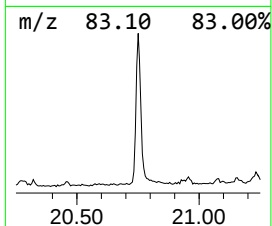
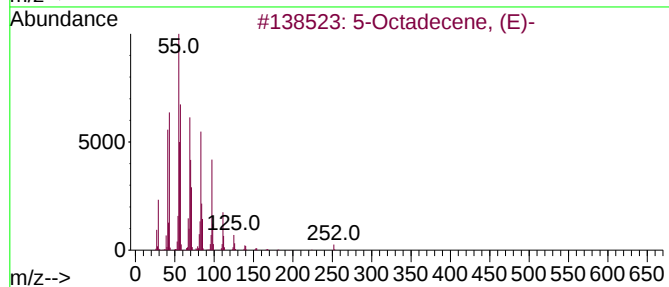
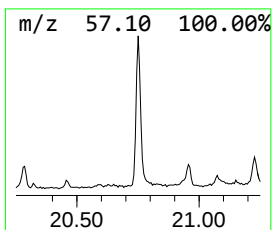
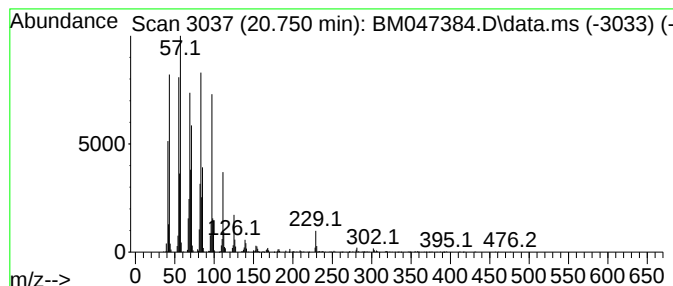
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Octadecene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.750	7.34 ng	1186320	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
5			Cyclotetradecane	196	C14H28	000295-17-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
Data File : BM047384.D
Acq On : 28 Aug 2024 17:05
Operator : RC/JU
Sample : P3767-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P-1-COMPOSITE

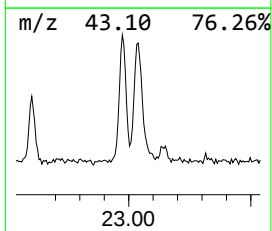
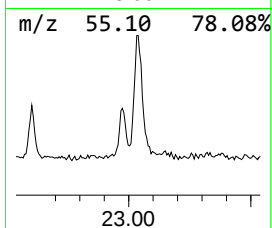
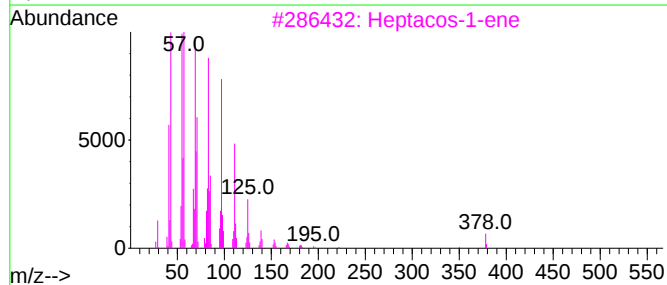
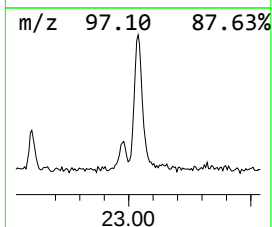
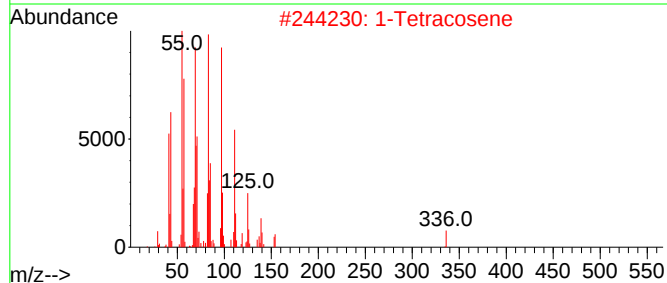
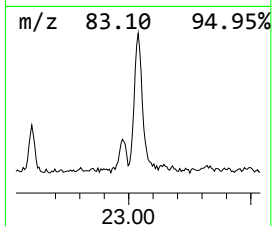
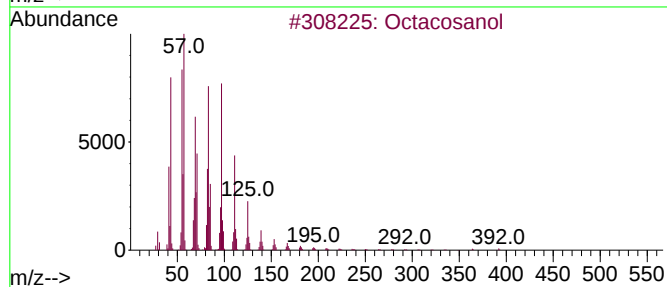
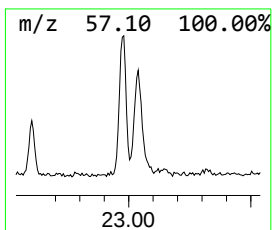
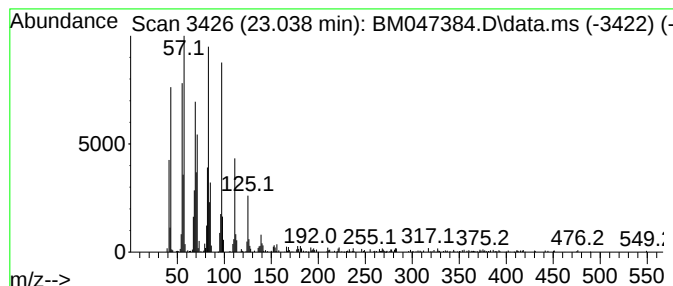
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.038	4.68 ng	633992	Perylene-d12	23.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	94
2			1-Tetracosene	336	C24H48	010192-32-2	93
3			Heptacos-1-ene	378	C27H54	015306-27-1	93
4			Pentacos-1-ene	350	C25H50	016980-85-1	93
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082824\
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Sample : P3767-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P-1-COMPOSITE

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.257	3.257	2.1	ng	188580	1	7.345	1785340	20.0
2-Pentanone, 4-...	4.557	3.9	ng	347518	1	7.345	1785340	20.0
1-Phenoxypropan...	10.869	3.4	ng	421854	2	10.104	2459920	20.0
n-Hexadecanoic ...	17.715	8.5	ng	1558660	4	16.774	3657900	20.0
Octadecanoic acid	19.015	3.7	ng	603294	5	21.021	3230430	20.0
5-Octadecene, (E)-	20.750	7.3	ng	1186320	5	21.021	3230430	20.0
Octacosanol	23.038	4.7	ng	633992	6	23.721	2707970	20.0