

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
 Data File : BF138286.D
 Acq On : 21 Jun 2024 15:28
 Operator : CG\JU
 Sample : P2977-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OSTL-A5

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-BF061224.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138286.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	9	14	20	rVB	1736186	2162266	56.20%	6.856%
2	3.387	218	221	236	rBV	37272	84052	2.18%	0.267%
3	5.093	508	511	517	rVB	170841	189694	4.93%	0.601%
4	5.498	576	580	583	rBV	3347793	2981535	77.49%	9.454%
5	5.828	631	636	643	rBV	54463	51465	1.34%	0.163%
6	6.504	747	751	754	rBV	3165407	3006052	78.13%	9.532%
7	6.881	812	815	819	rVB	2027286	1608388	41.80%	5.100%
8	7.439	906	910	913	rBV	2204508	1948988	50.65%	6.180%
9	7.692	950	953	957	rBV	126126	100567	2.61%	0.319%
10	8.163	1029	1033	1036	rBV	2713464	2120256	55.10%	6.723%
11	8.475	1082	1086	1095	rBV	110298	131787	3.43%	0.418%
12	9.239	1212	1216	1219	rBV	4782760	3847688	100.00%	12.201%
13	9.916	1327	1331	1343	rBV	2749572	2295588	59.66%	7.279%
14	10.010	1343	1347	1353	rVB2	46951	65553	1.70%	0.208%
15	10.704	1461	1465	1479	rBV	2048450	1799609	46.77%	5.706%
16	11.404	1580	1584	1587	rBV	2105716	1759650	45.73%	5.580%
17	11.927	1670	1673	1685	rVB	198199	216603	5.63%	0.687%
18	12.610	1786	1789	1792	rBV	64805	64616	1.68%	0.205%
19	12.710	1803	1806	1817	rBV4	42544	56926	1.48%	0.181%
20	12.839	1824	1828	1834	rVB	63175	62514	1.62%	0.198%
21	12.986	1849	1853	1856	rBV	3339368	2665067	69.26%	8.451%
22	13.557	1939	1950	1957	rBV	16725	58756	1.53%	0.186%
23	13.892	2003	2007	2025	rBV8	55658	238548	6.20%	0.756%
24	14.039	2028	2032	2035	rBV	1663847	1442266	37.48%	4.573%
25	14.510	2109	2112	2115	rBV	61880	59166	1.54%	0.188%
26	14.898	2174	2178	2181	rBV	92058	93718	2.44%	0.297%
27	14.968	2186	2190	2197	rVB	214172	221348	5.75%	0.702%
28	15.074	2205	2208	2218	rBV	37646	81114	2.11%	0.257%
29	15.163	2219	2223	2226	rBV	100394	104306	2.71%	0.331%
30	15.215	2226	2232	2234	rBV4	71901	135384	3.52%	0.429%
31	15.510	2277	2282	2293	rVB	1100337	1349185	35.06%	4.278%
32	15.751	2319	2323	2333	rVB2	89827	135969	3.53%	0.431%
33	15.992	2359	2364	2370	rVB	88376	125087	3.25%	0.397%
34	16.804	2497	2502	2509	rVB4	50950	98426	2.56%	0.312%
35	17.109	2550	2554	2560	rVB6	22709	45619	1.19%	0.145%
36	18.174	2729	2735	2746	rVB8	42501	129269	3.36%	0.410%

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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_F\Methods\8270-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

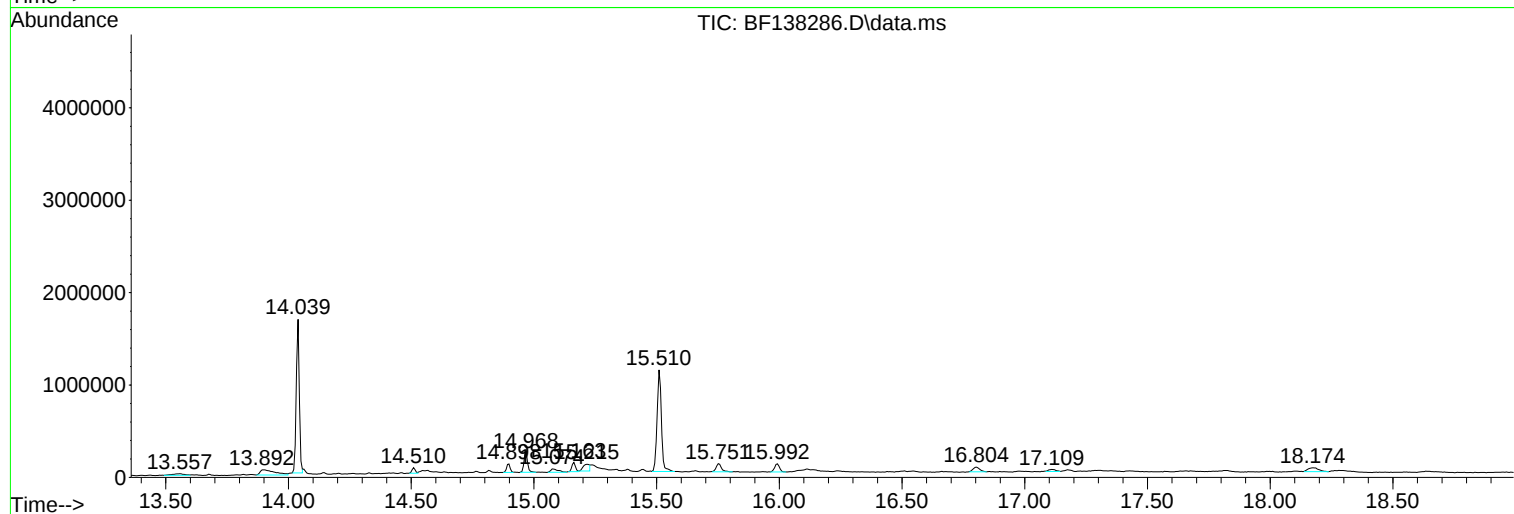
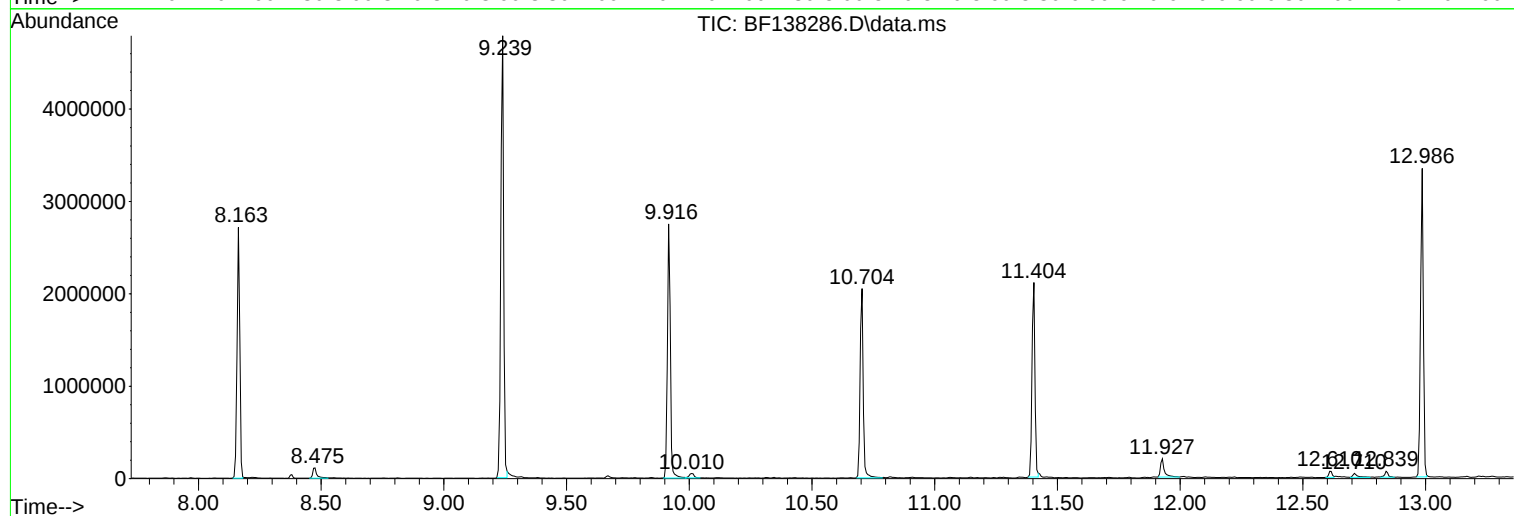
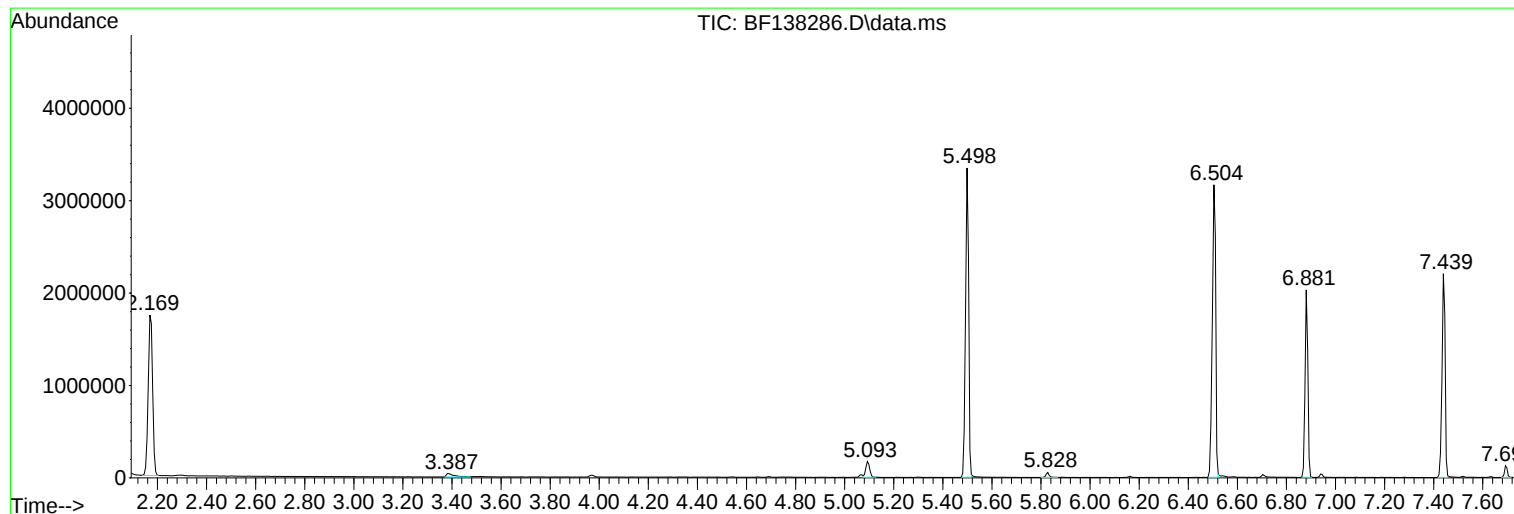
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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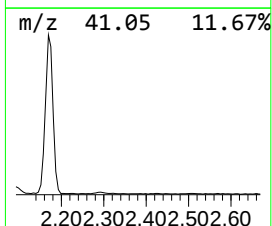
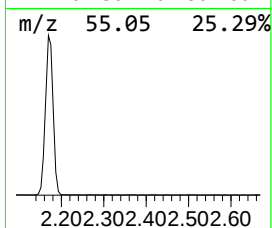
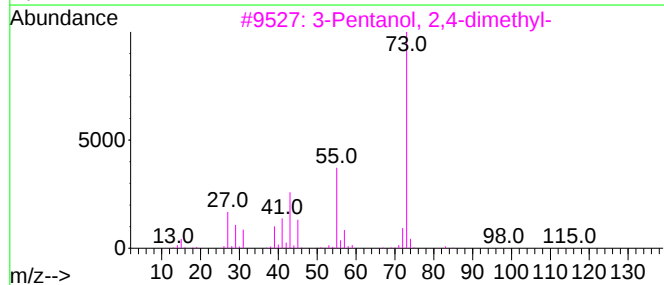
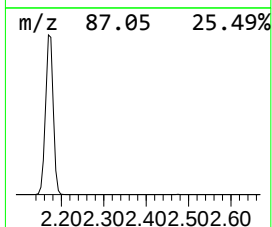
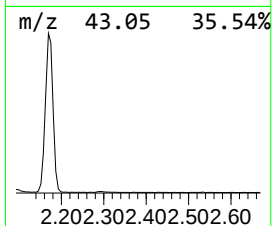
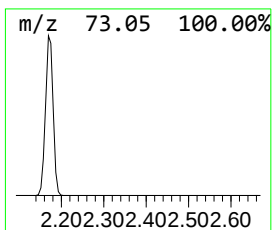
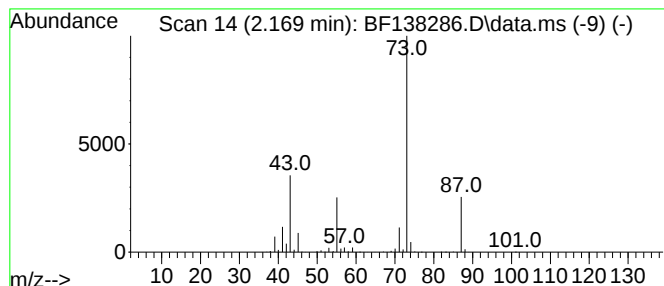
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	26.89 ng	2162270	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	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23



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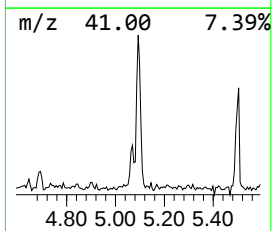
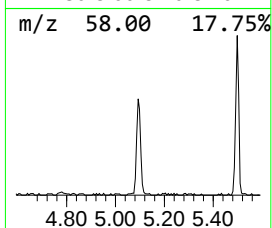
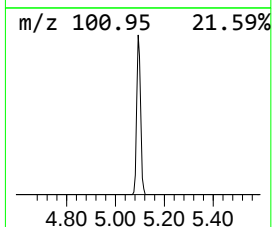
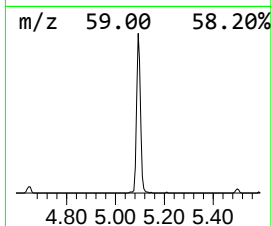
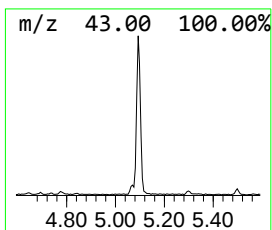
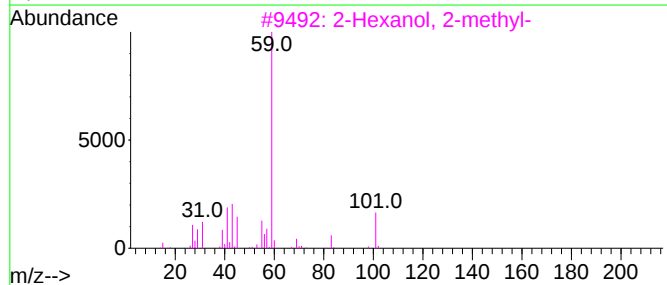
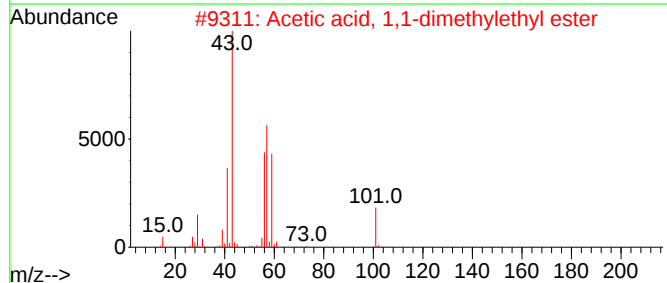
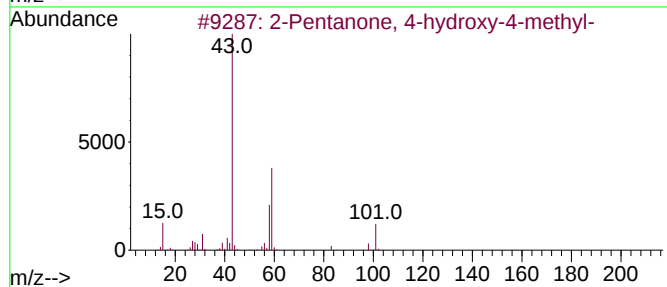
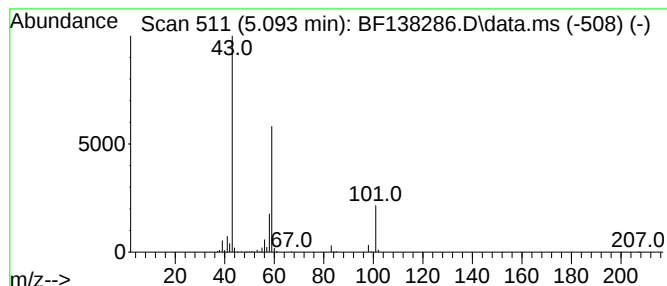
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	2.36 ng	189694	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	Guanidine	59	CH5N3	000113-00-8	9		



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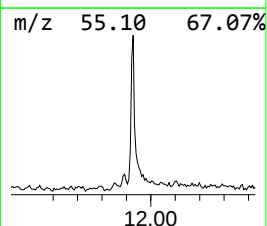
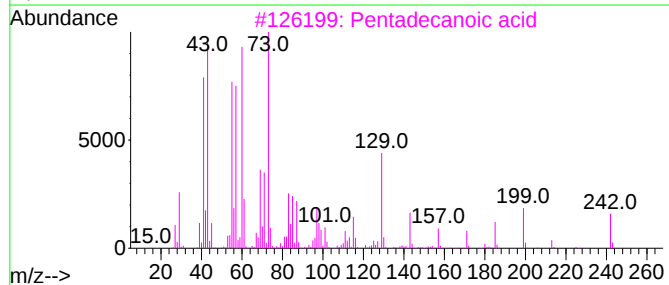
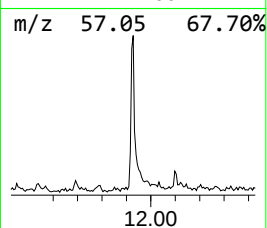
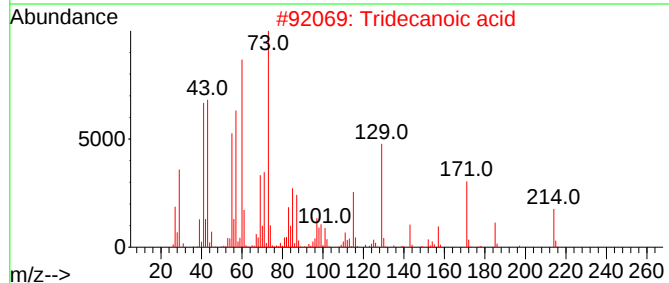
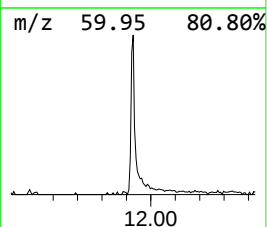
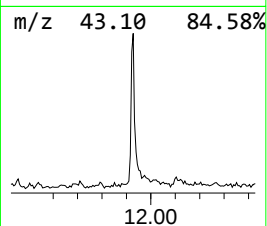
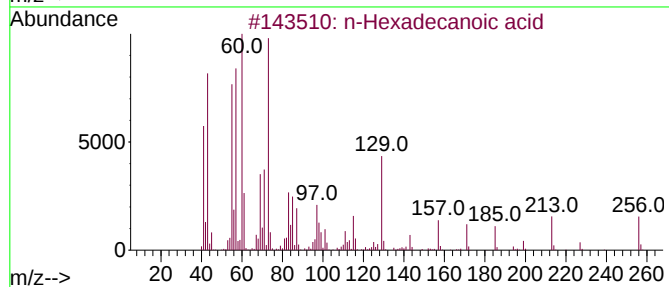
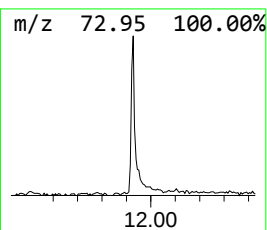
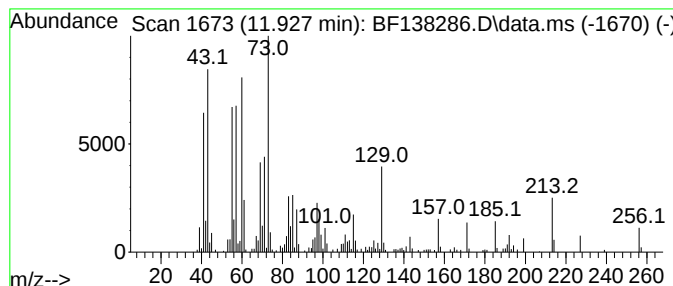
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	2.46 ng	216603	Phenanthrene-d10	11.404

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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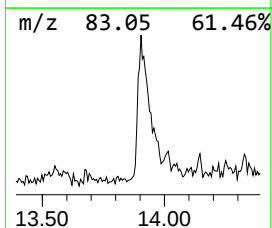
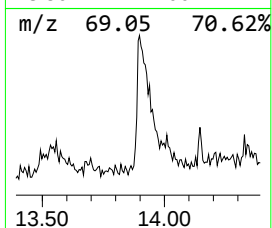
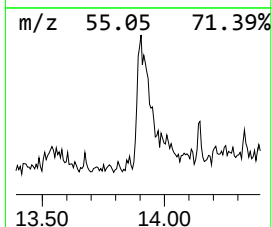
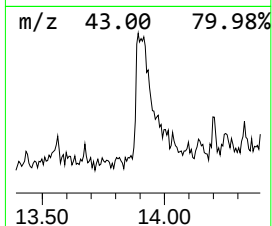
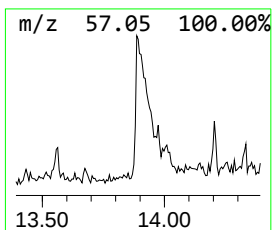
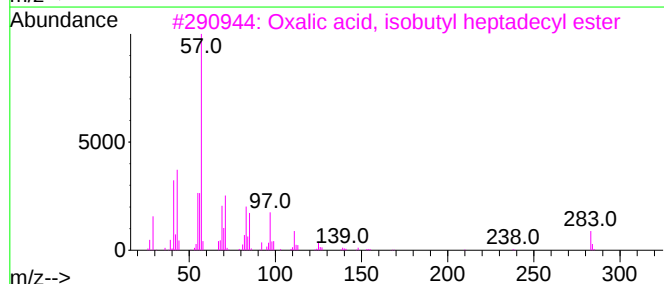
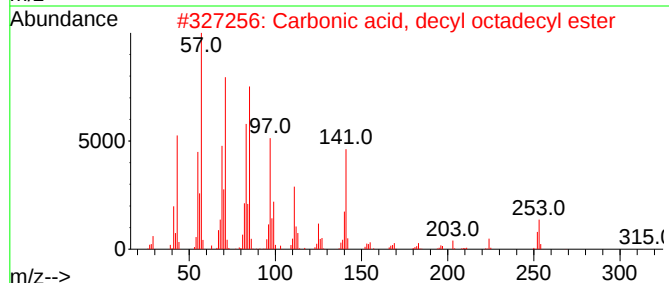
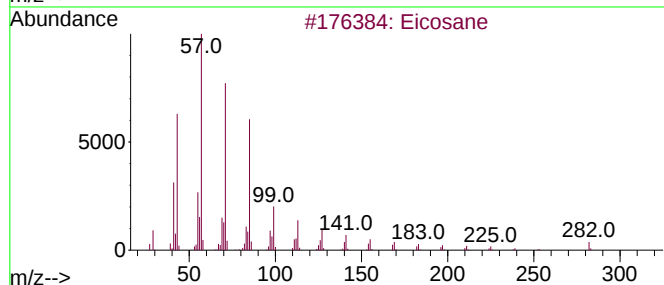
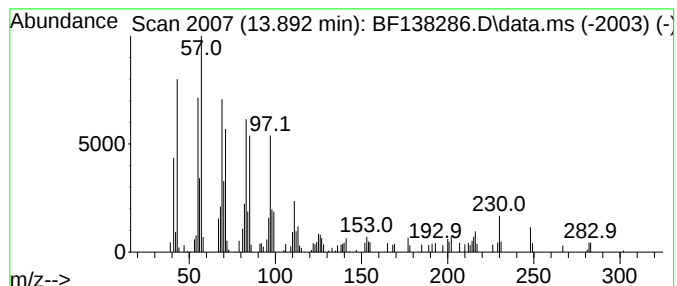
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.31 ng	238548	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	83
2	Carbonic acid, decyl octadecyl e...			454	C29H58O3	1000383-16-7	74
3	Oxalic acid, isobutyl heptadecyl...			384	C23H44O4	1000309-38-2	62
4	Tetratriacontyl pentafluoropropi...			641	C37H69F5O2	1000351-81-5	62
5	Triacontyl pentafluoropropionate			584	C33H61F5O2	1000351-80-0	62



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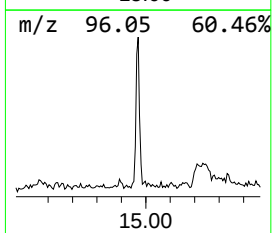
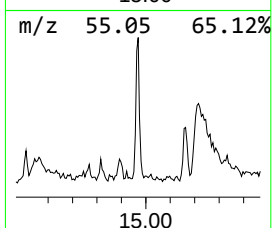
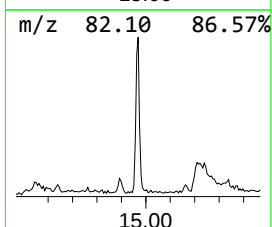
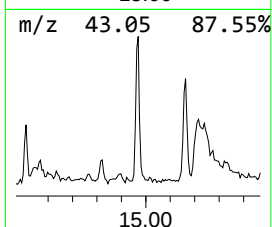
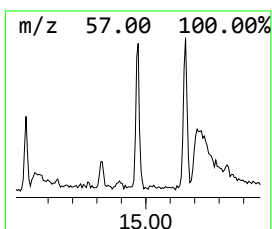
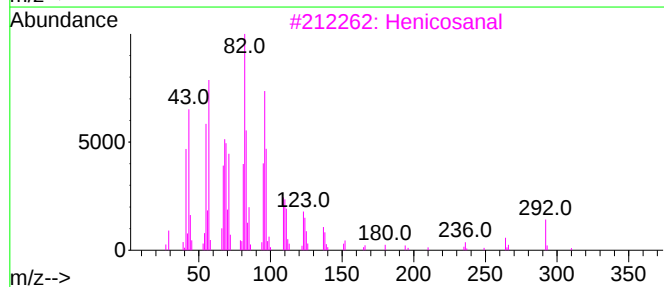
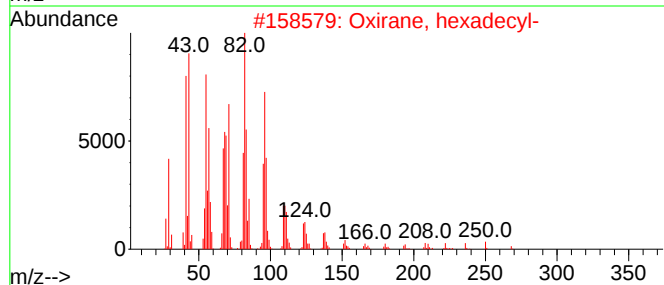
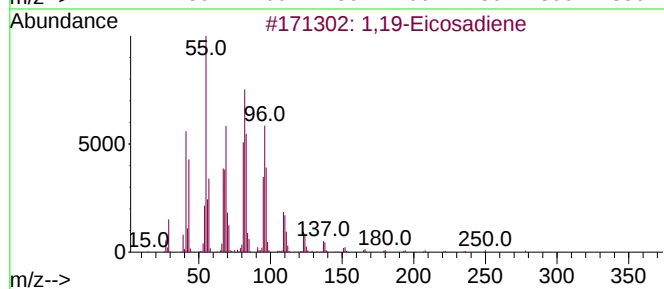
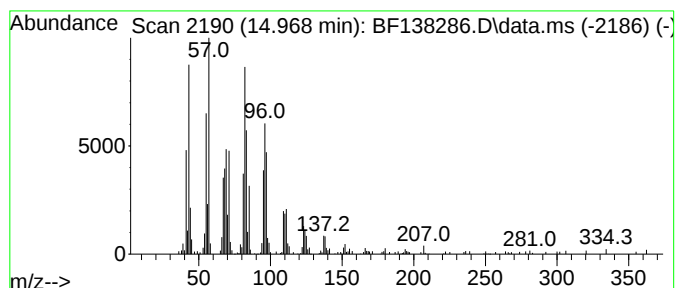
Instrument :
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ClientSampleId :
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Peak Number 5 1,19-Eicosadiene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.968	3.28 ng	221348	Perylene-d12	15.509	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	95
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	93
3	Henicosanal	310	C21H42O	051227-32-8	91
4	Octadecanal	268	C18H36O	000638-66-4	91
5	Eicosanal-	296	C20H40O	002400-66-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061224\
Data File : BF138286.D
Acq On : 21 Jun 2024 15:28
Operator : CG\JU
Sample : P2977-05
Misc :
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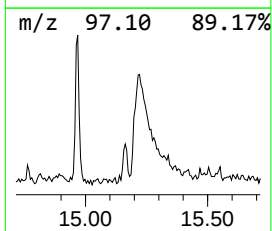
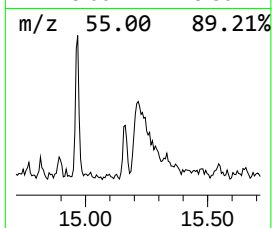
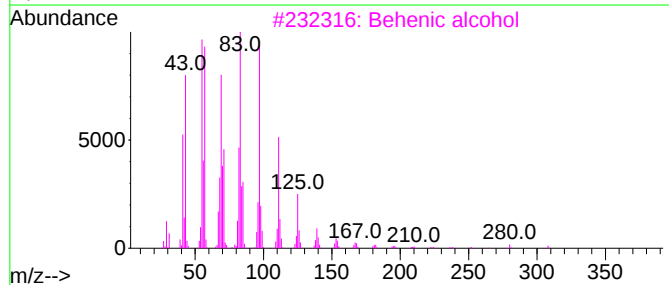
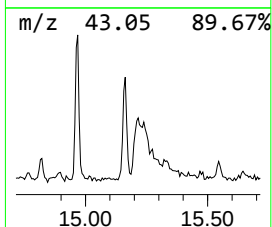
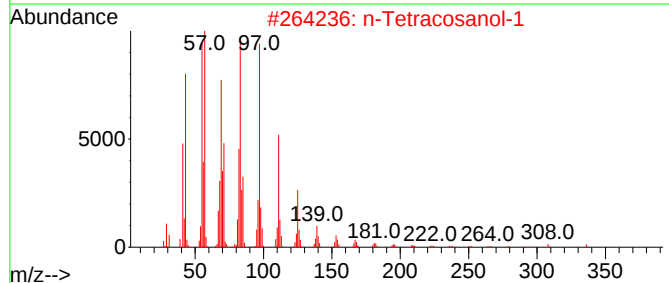
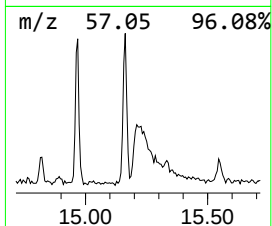
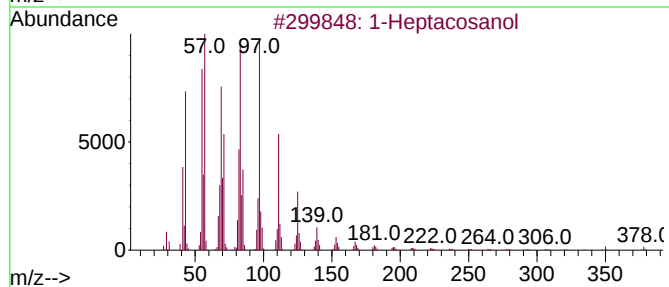
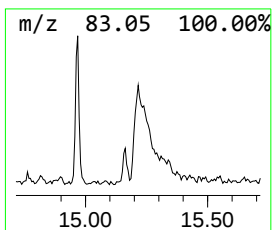
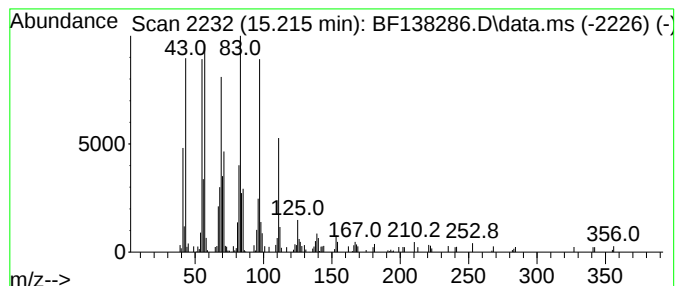
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ClientSampleId :
OSTL-A5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.215	2.01 ng	135384	Perylene-d12		15.509	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Heptacosanol		396	C27H56O	002004-39-9	91
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	91
3	Behenic alcohol		326	C22H46O	000661-19-8	91
4	Octacosanol		410	C28H58O	000557-61-9	90
5	1-Pentadecene		210	C15H30	013360-61-7	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138286.D
Acq On : 21 Jun 2024 15:28
Operator : CG\JU
Sample : P2977-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A5

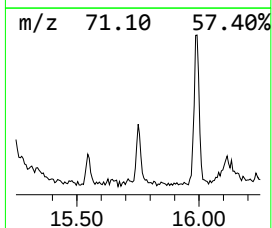
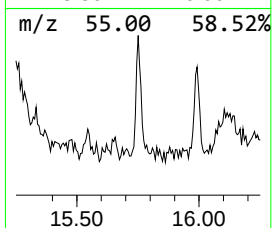
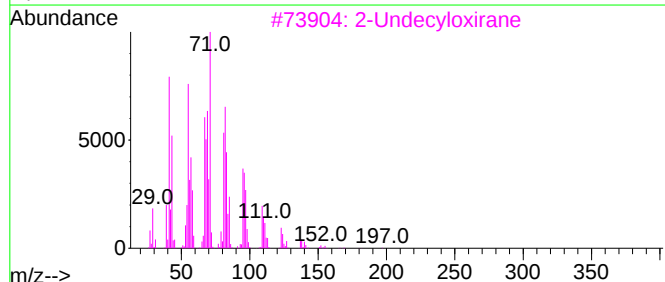
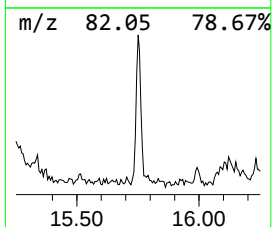
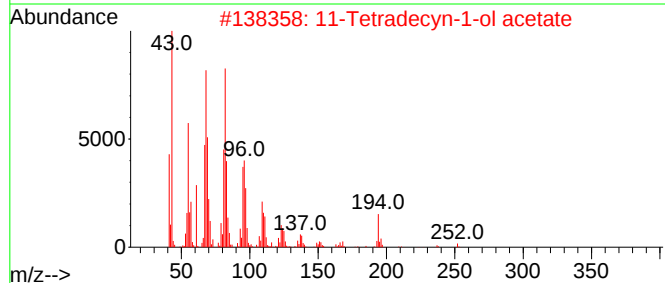
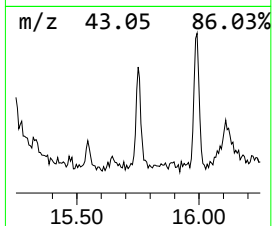
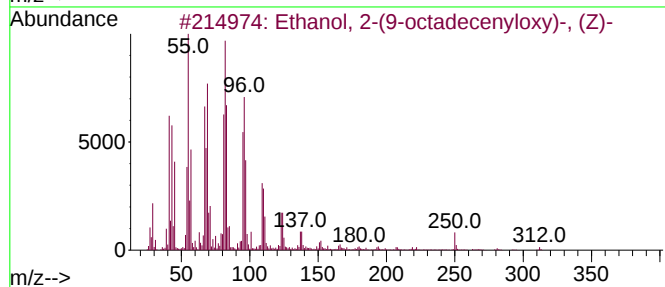
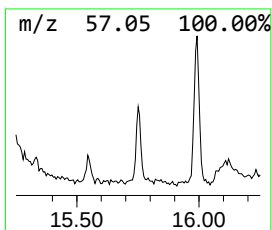
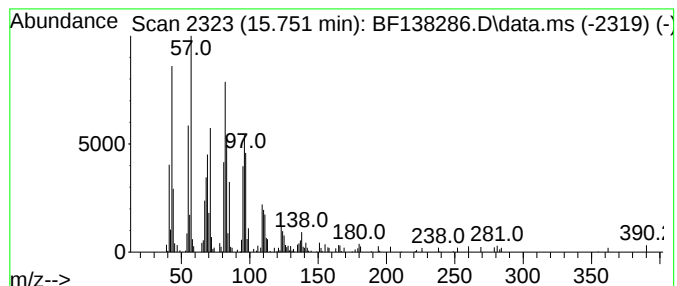
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Ethanol, 2-(9-octadecenylox... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	2.02 ng	135969	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(9-octadecenyloxy)-, ...	312	C20H40O2	005353-25-3	81
2			11-Tetradecyn-1-ol acetate	252	C16H28O2	033925-72-3	76
3			2-Undecyloxirane	198	C13H26O	001713-31-1	72
4			(Z)-Tetradec-11-en-1-yl 2,2,2-tr...	308	C16H27F3O2	1000385-85-4	72
5			16-Heptadecenal	252	C17H32O	1010144-57-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138286.D
Acq On : 21 Jun 2024 15:28
Operator : CG\JU
Sample : P2977-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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
Butane, 2-metho...	2.169	26.9	ng	2162270	1	6.881	1608390	20.0
2-Pentanone, 4-...	5.093	2.4	ng	189694	1	6.881	1608390	20.0
n-Hexadecanoic ...	11.927	2.5	ng	216603	4	11.404	1759650	20.0
Eicosane	13.892	3.3	ng	238548	5	14.039	1442270	20.0
1,19-Eicosadiene	14.968	3.3	ng	221348	6	15.509	1349190	20.0
1-Heptacosanol	15.215	2.0	ng	135384	6	15.509	1349190	20.0
Ethanol, 2-(9-o...	15.751	2.0	ng	135969	6	15.509	1349190	20.0