

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
 Data File : BF140265.D
 Acq On : 07 Nov 2024 10:55
 Operator : RC/JU
 Sample : P4693-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BP-G4-WC

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-BF110524.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140265.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	4	12	19	rVB	1797225	2820081	66.44%	8.585%
2	2.269	24	30	38	rBV	54133	84893	2.00%	0.258%
3	3.969	313	319	326	rBV	27875	42946	1.01%	0.131%
4	5.104	500	512	521	rBV	82271	131063	3.09%	0.399%
5	5.492	572	578	584	rBV	2440541	3362470	79.22%	10.236%
6	6.498	742	749	754	rBV	2533909	3538534	83.37%	10.772%
7	6.875	808	813	818	rVB	651708	785208	18.50%	2.390%
8	7.433	902	908	913	rBV	1712592	2283336	53.79%	6.951%
9	7.686	946	951	959	rVB	48913	62042	1.46%	0.189%
10	8.157	1025	1031	1039	rBV	804487	1015580	23.93%	3.092%
11	8.369	1063	1067	1070	rBV	51478	74276	1.75%	0.226%
12	9.233	1207	1214	1219	rBV	3066347	4024327	94.81%	12.251%
13	9.916	1324	1330	1335	rBV	904567	1181047	27.82%	3.595%
14	10.627	1446	1451	1458	rBV	321678	399094	9.40%	1.215%
15	10.704	1458	1464	1478	rBV	2195782	2865573	67.51%	8.724%
16	11.404	1578	1583	1590	rBV	983697	1242337	29.27%	3.782%
17	11.469	1590	1594	1598	rVB2	37282	46391	1.09%	0.141%
18	11.933	1665	1673	1685	rBV	365252	603060	14.21%	1.836%
19	12.621	1785	1790	1800	rBV3	16956	44016	1.04%	0.134%
20	12.716	1801	1806	1815	rBV	82513	143427	3.38%	0.437%
21	12.992	1847	1853	1859	rBV	3213282	4244606	100.00%	12.922%
22	13.563	1946	1950	1959	rVB2	32460	52397	1.23%	0.160%
23	13.904	2002	2008	2026	rBV	147323	344243	8.11%	1.048%
24	14.057	2028	2034	2042	rVV	697068	924489	21.78%	2.814%
25	14.227	2059	2063	2075	rVB	41437	66702	1.57%	0.203%
26	14.492	2094	2108	2132	rBV3	286439	1405809	33.12%	4.280%
27	14.845	2163	2168	2178	rBV3	97119	202033	4.76%	0.615%
28	14.945	2181	2185	2192	rVV	29103	48684	1.15%	0.148%
29	15.568	2285	2291	2304	rBV	488243	809755	19.08%	2.465%

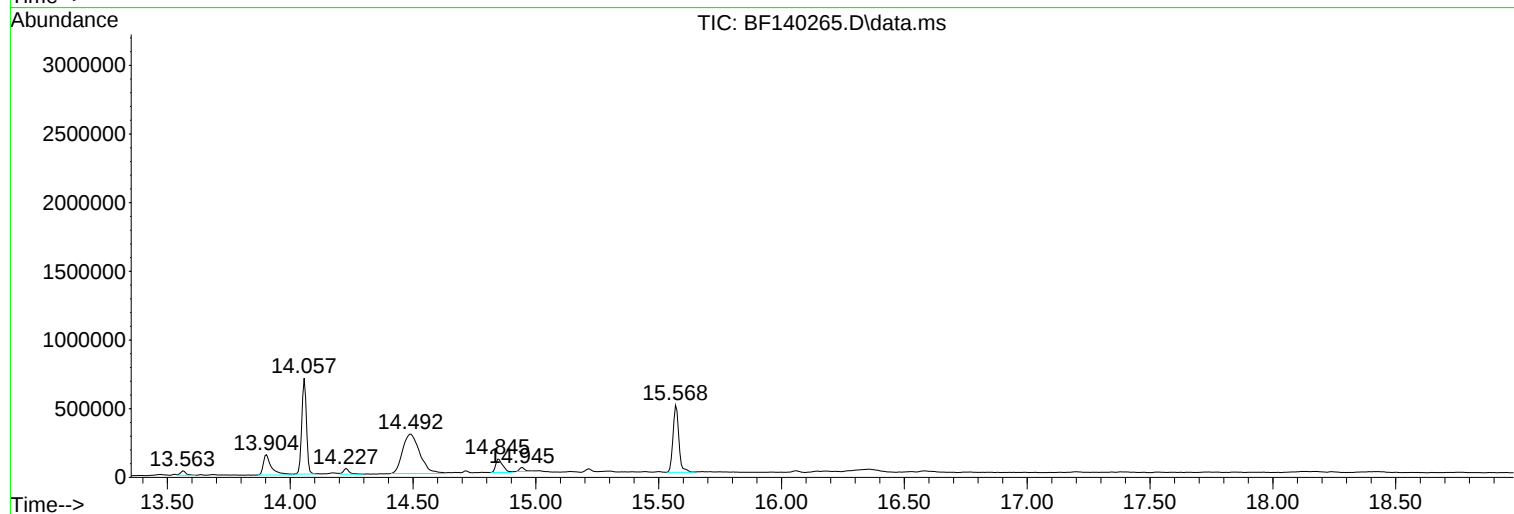
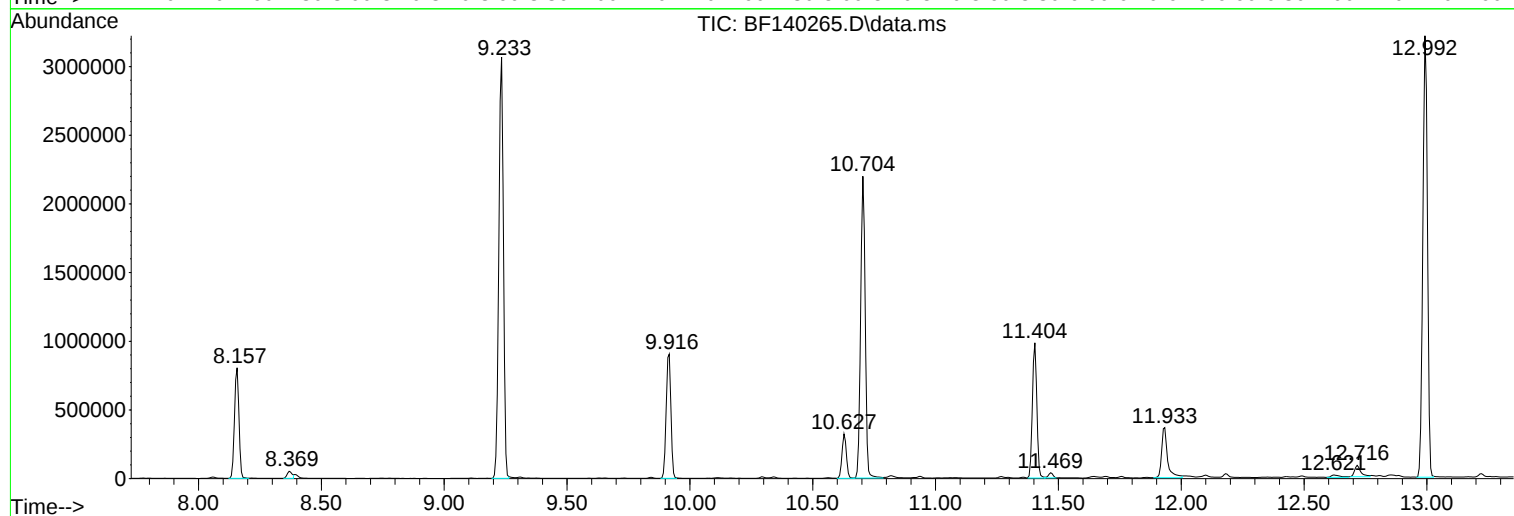
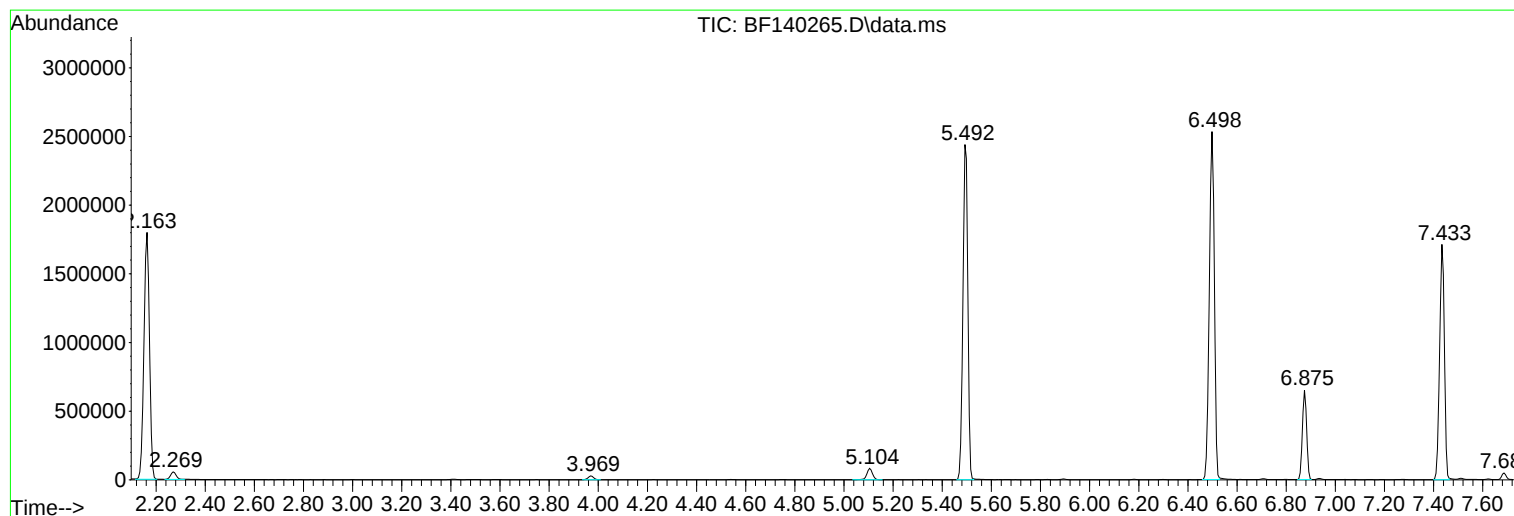
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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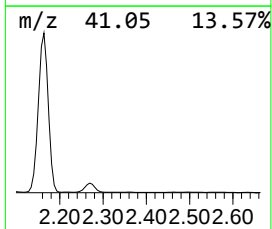
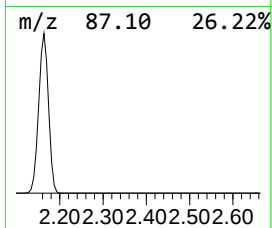
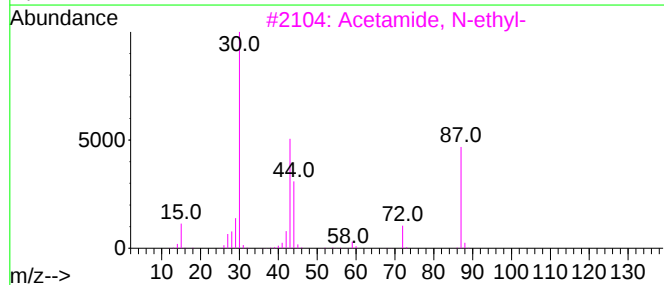
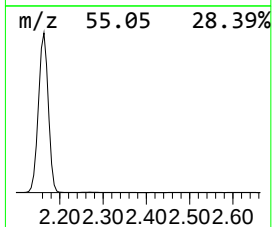
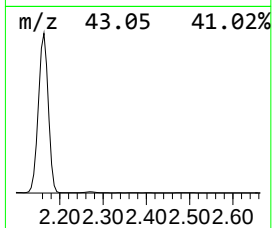
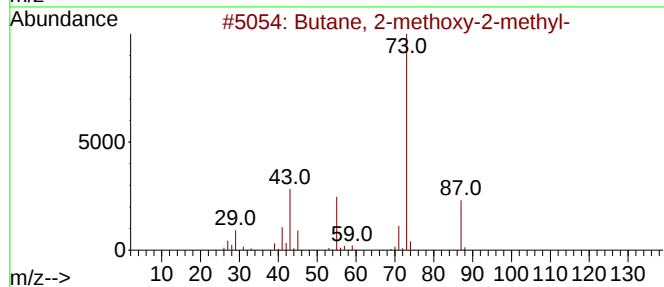
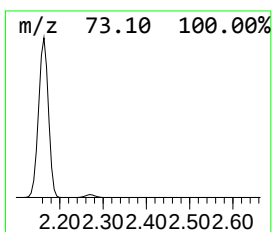
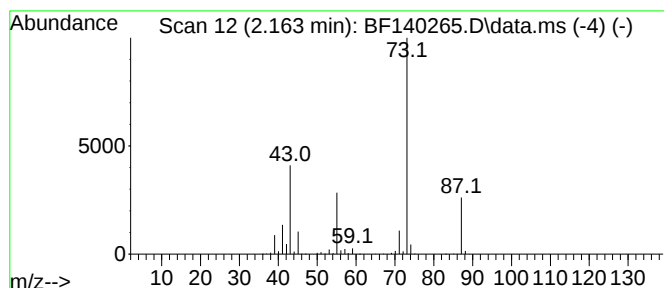
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	71.83 ng	2820080	1,4-Dichlorobenzene-d4	6.875

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	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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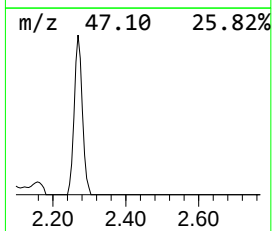
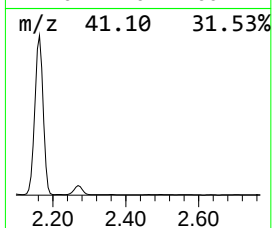
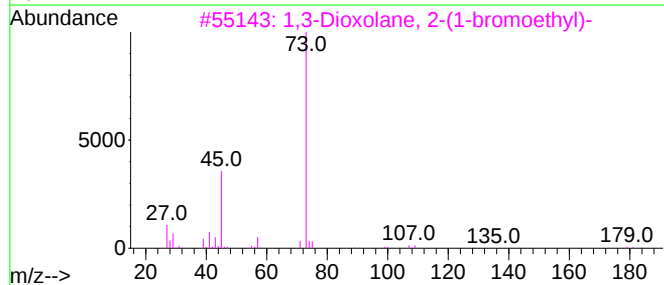
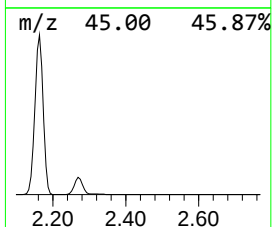
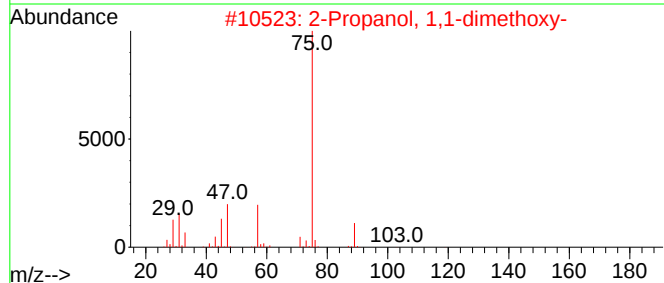
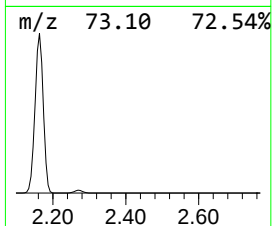
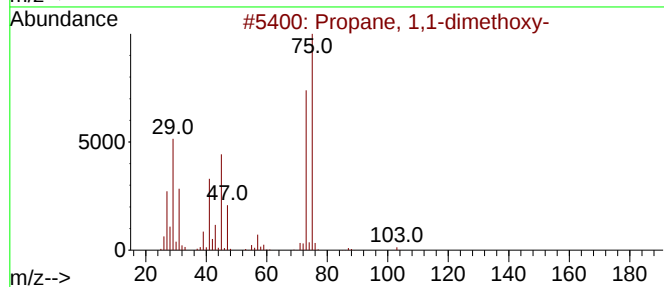
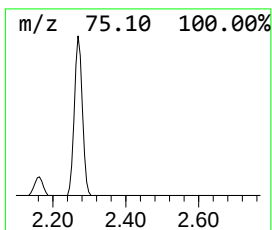
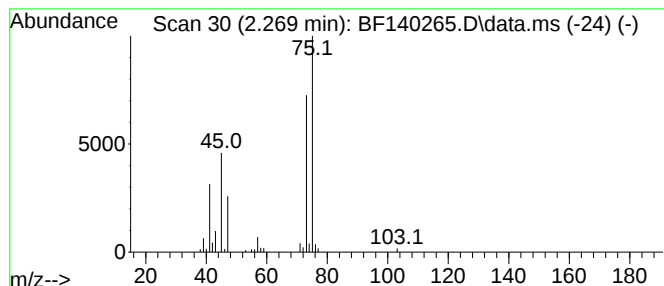
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	2.16 ng	84893	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	42
3			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	22
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9



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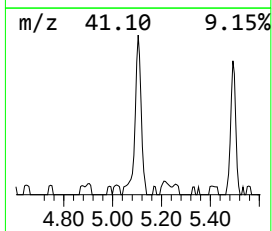
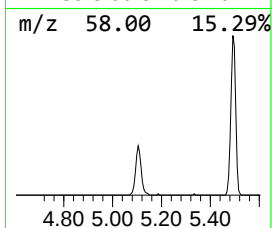
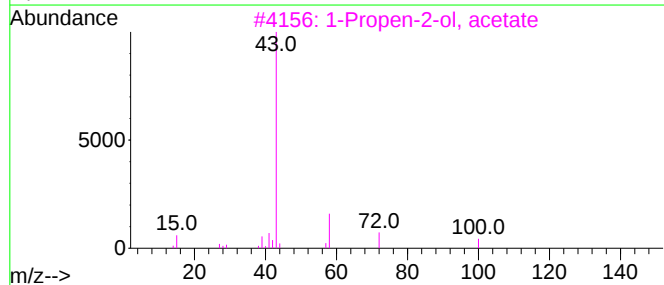
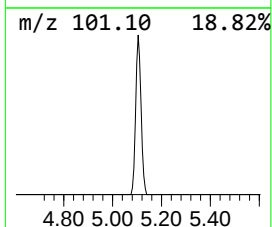
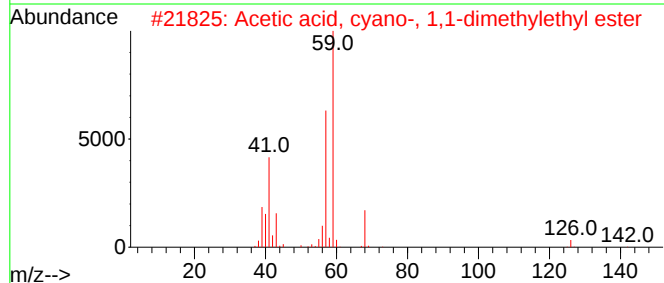
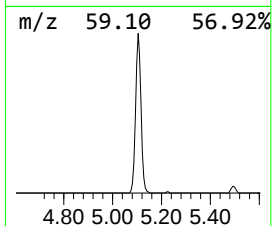
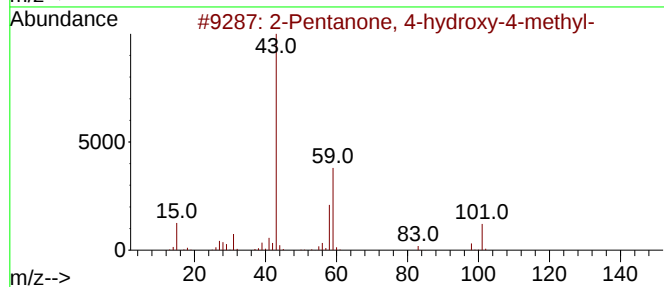
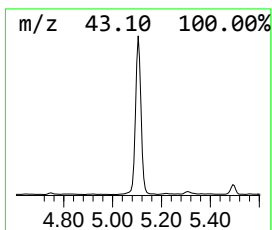
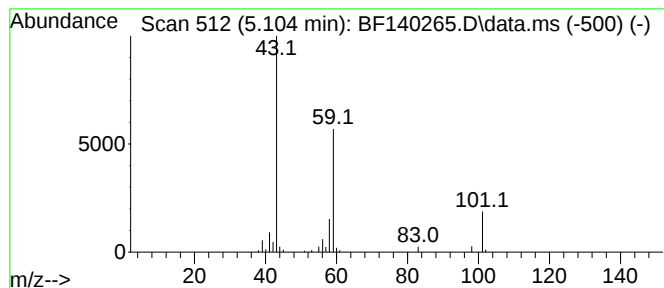
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	3.34 ng	131063	1,4-Dichlorobenzene-d4	6.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	



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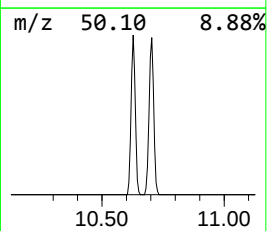
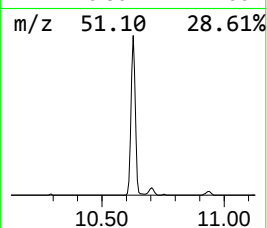
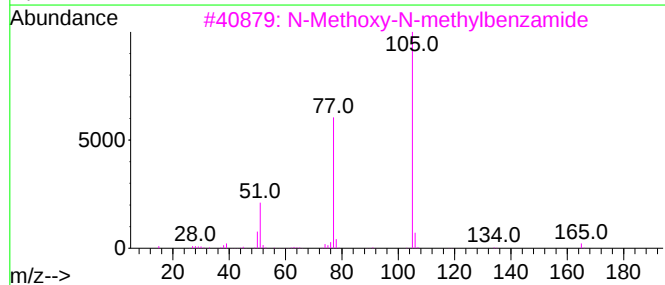
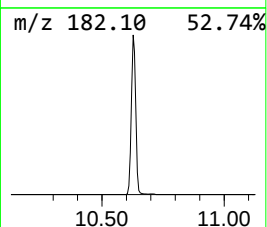
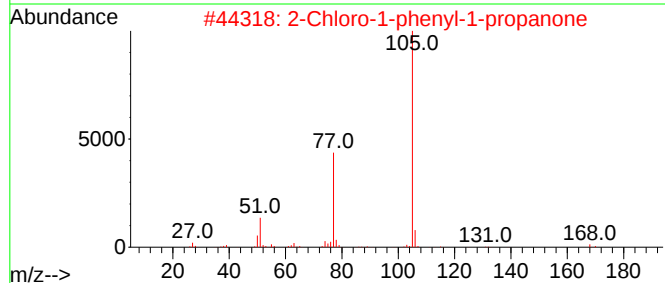
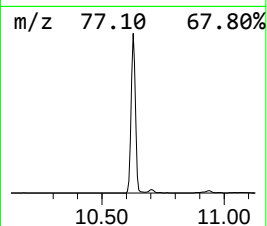
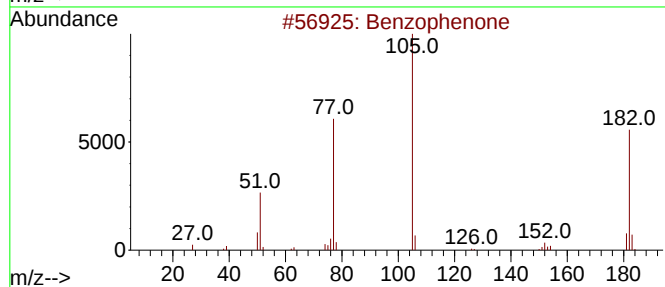
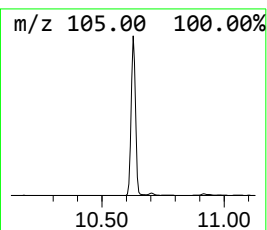
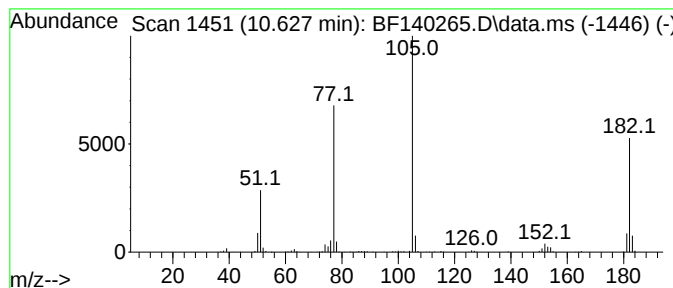
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Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.627	6.76 ng	399094	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	47
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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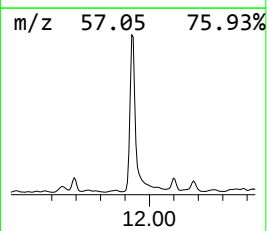
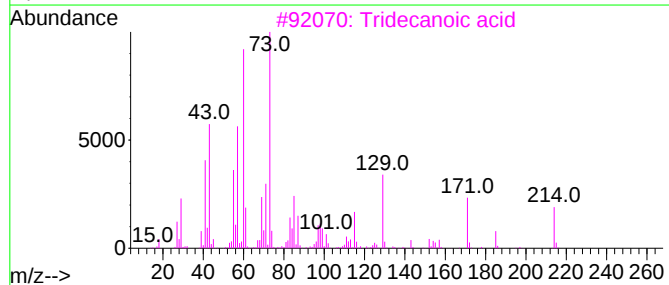
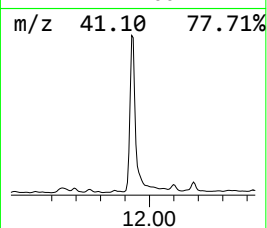
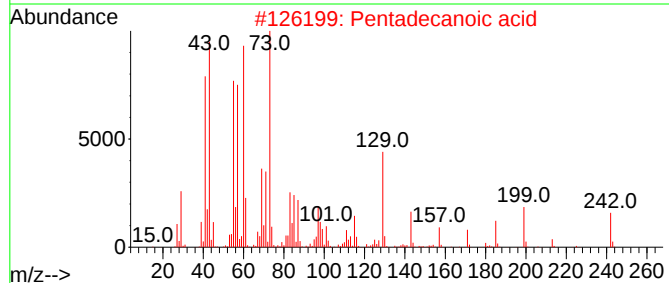
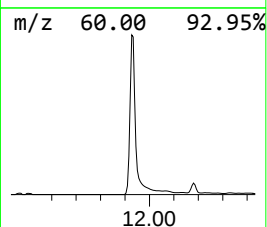
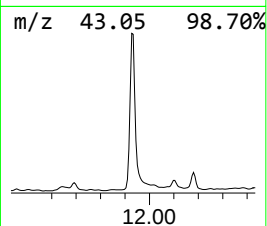
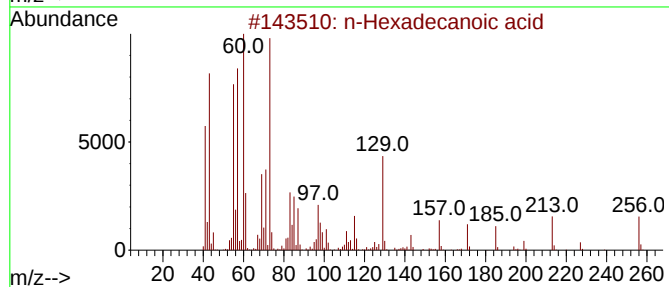
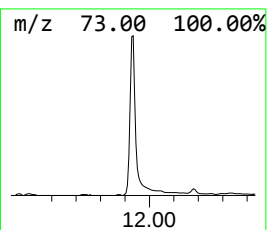
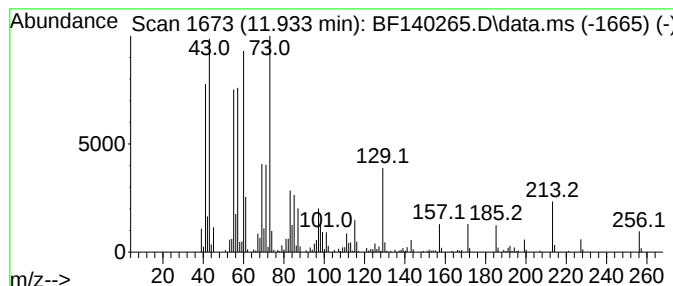
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	9.71 ng	603060	Phenanthrene-d10	11.404

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	91
4			n-Decanoic acid	172	C10H20O2	000334-48-5	68
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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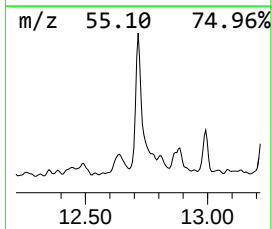
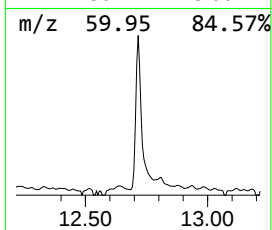
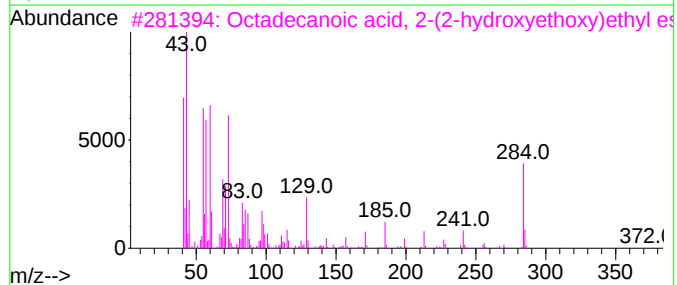
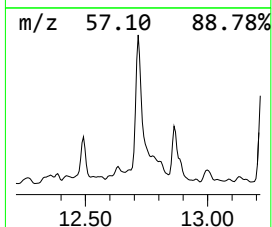
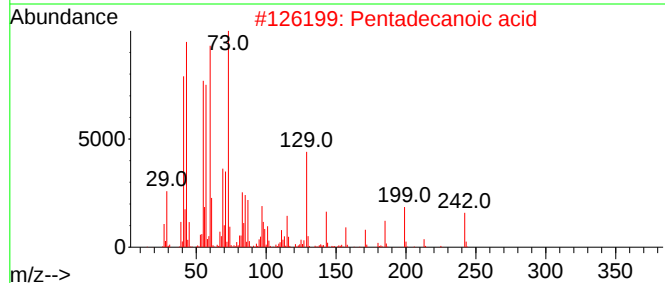
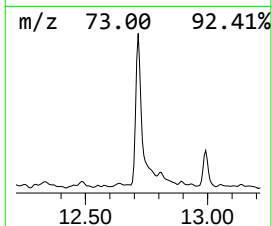
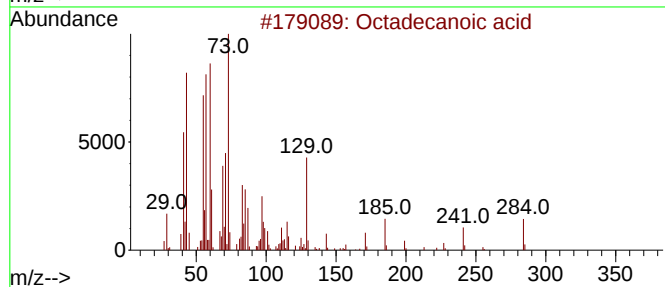
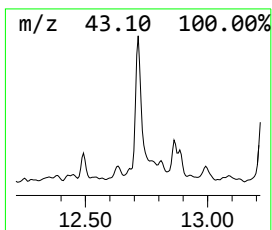
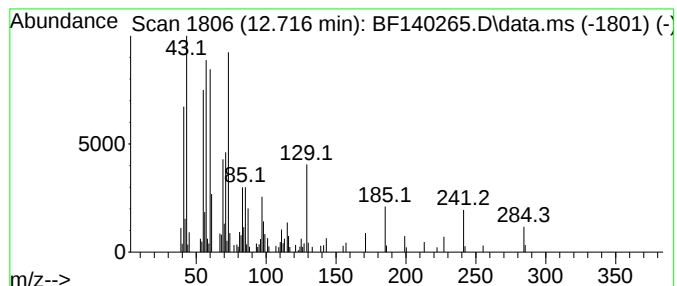
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.31 ng	143427	Phenanthrene-d10	11.404

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	87
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140265.D
Acq On : 07 Nov 2024 10:55
Operator : RC/JU
Sample : P4693-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-G4-WC

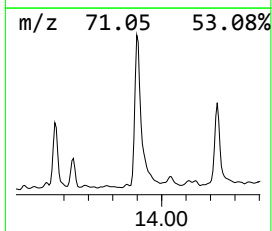
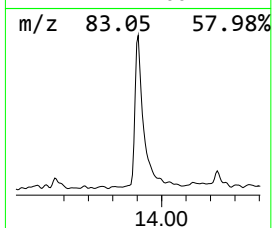
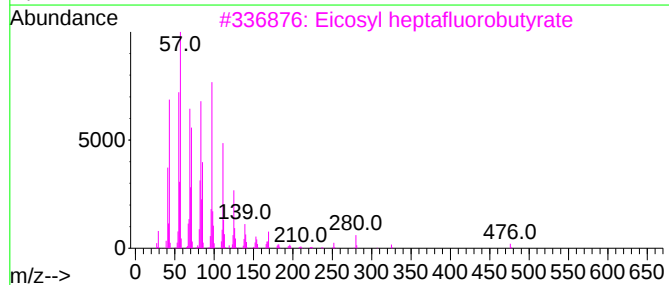
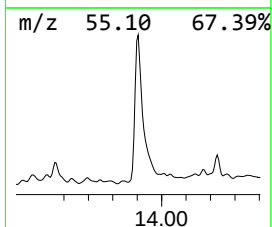
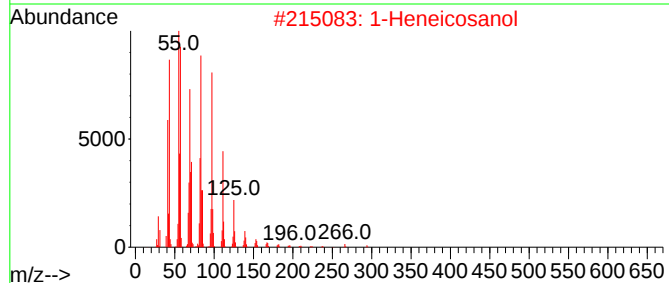
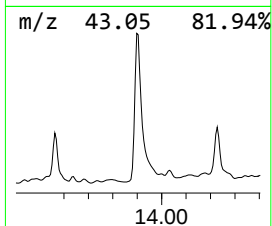
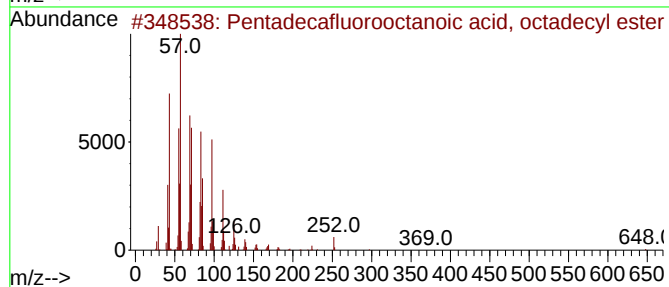
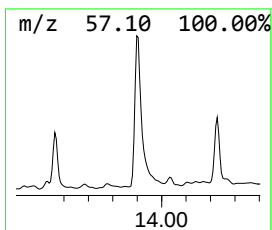
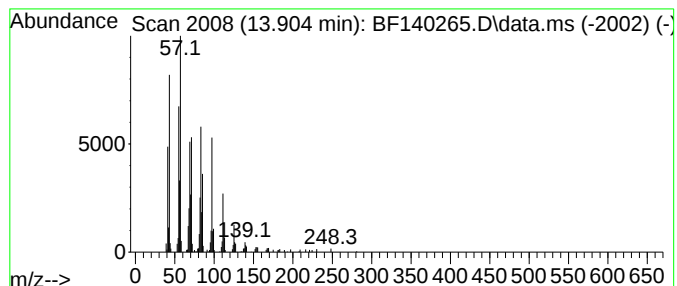
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	7.45 ng	344243	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
4			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
5			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140265.D
Acq On : 07 Nov 2024 10:55
Operator : RC/JU
Sample : P4693-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-G4-WC

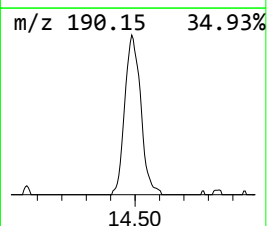
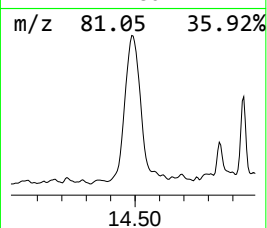
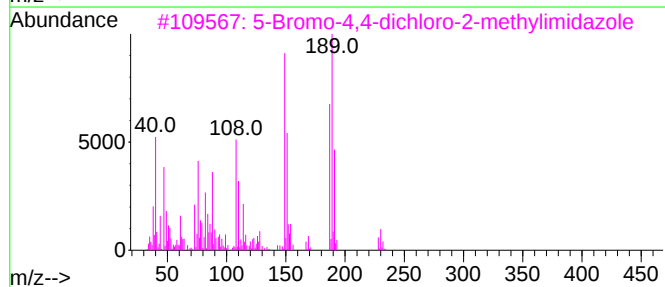
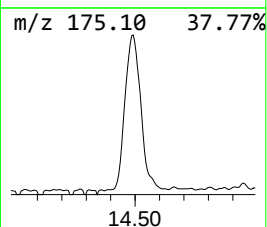
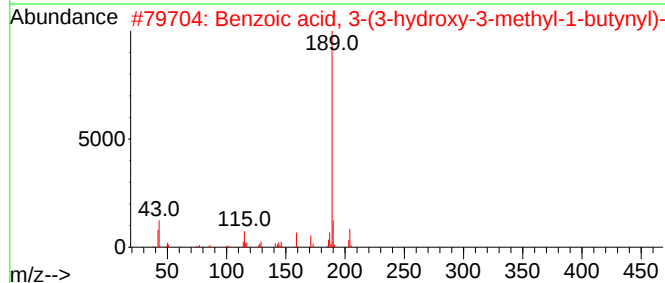
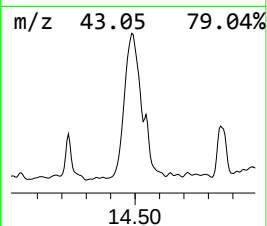
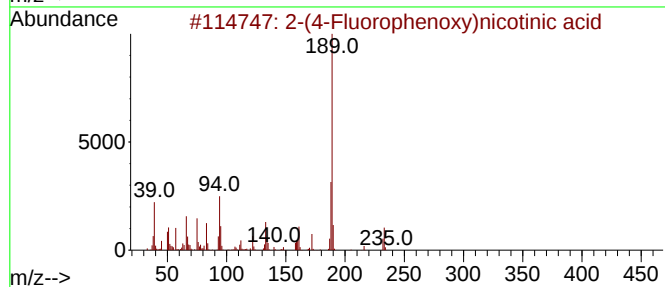
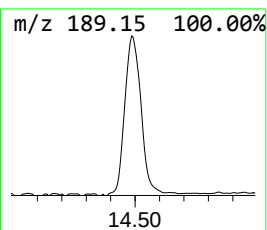
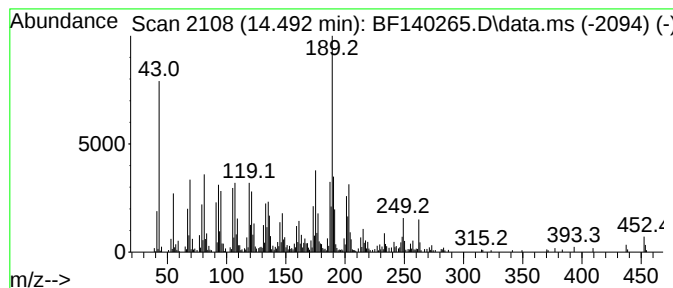
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.492 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	30.41 ng	1405810	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Fluorophenoxy)nicotinic acid	233	C12H8FN03	054629-13-9	43		
2	Benzoic acid, 3-(3-hydroxy-3-met...	204	C12H12O3	1000337-06-2	41		
3	5-Bromo-4,4-dichloro-2-methylimi...	228	C4H3BrCl2N2	1000409-98-8	38		
4	1,2-Dicarbadoecaborane(12), 1-[...	234	C6H20B10S	062906-36-9	38		
5	1H-[1,4]Oxazino[4,3-a][1,3]benzi...	189	C10H11N3O	1000362-54-6	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140265.D
Acq On : 07 Nov 2024 10:55
Operator : RC/JU
Sample : P4693-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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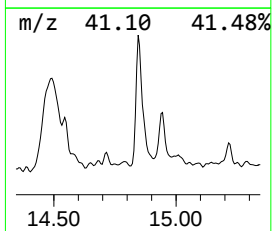
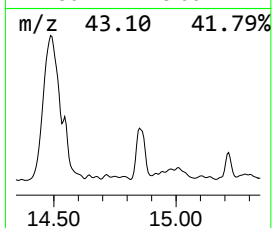
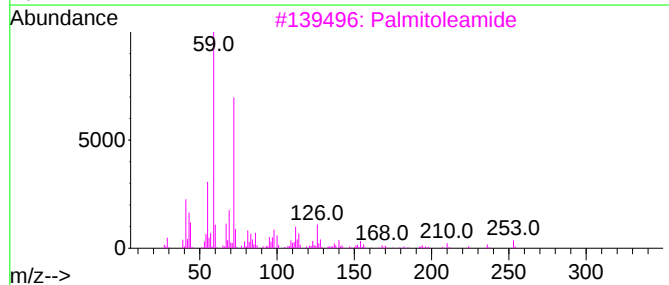
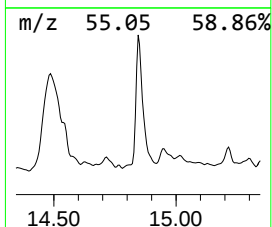
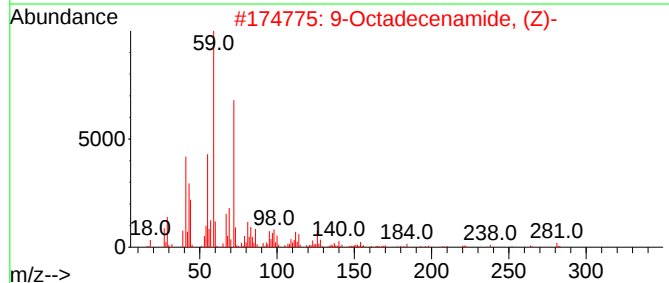
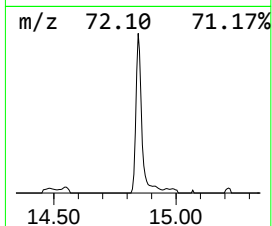
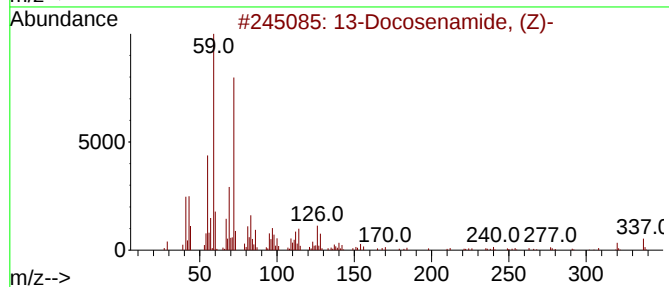
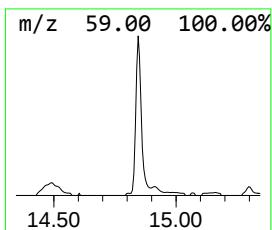
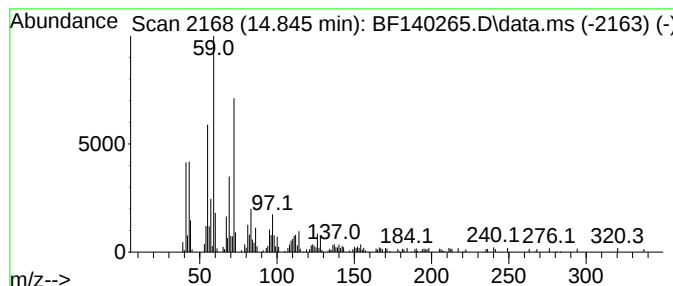
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	4.99 ng	202033	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	94
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
3			Palmitoleamide	253	C16H31NO	106010-22-4	62
4			Dodecanamide	199	C12H25NO	001120-16-7	53
5			Octadecanamide	283	C18H37NO	000124-26-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140265.D
Acq On : 07 Nov 2024 10:55
Operator : RC/JU
Sample : P4693-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-G4-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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...	2.163	71.8	ng	2820080	1	6.875	785208	20.0
Propane, 1,1-di...	2.269	2.2	ng	84893	1	6.875	785208	20.0
2-Pentanone, 4-...	5.104	3.3	ng	131063	1	6.875	785208	20.0
Benzophenone	10.627	6.8	ng	399094	3	9.916	1181050	20.0
n-Hexadecanoic ...	11.933	9.7	ng	603060	4	11.404	1242340	20.0
Octadecanoic acid	12.716	2.3	ng	143427	4	11.404	1242340	20.0
Pentadecafluoro...	13.904	7.5	ng	344243	5	14.057	924489	20.0
unknown14.492	14.492	30.4	ng	1405810	5	14.057	924489	20.0
13-Docosenamide...	14.845	5.0	ng	202033	6	15.568	809755	20.0