

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112724\
 Data File : BF140667.D
 Acq On : 27 Nov 2024 14:04
 Operator : RC/JU
 Sample : P4985-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-756-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-BF112124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140667.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	3	10	20	rVB	575015	906766	42.85%	6.053%
2	5.498	574	579	602	rBV	1159487	1554035	73.44%	10.373%
3	6.504	745	750	768	rBV	1185393	1639798	77.50%	10.946%
4	6.869	807	812	819	rBV	344325	417295	19.72%	2.786%
5	7.433	902	908	918	rBV	783189	1054958	49.86%	7.042%
6	7.686	946	951	968	rBV2	18896	42421	2.00%	0.283%
7	8.151	1024	1030	1044	rBV	413186	542838	25.65%	3.624%
8	9.222	1207	1212	1222	rBV	1601445	2061424	97.42%	13.760%
9	9.904	1323	1328	1343	rBV	497044	651108	30.77%	4.346%
10	10.616	1444	1449	1456	rBV	137381	183291	8.66%	1.223%
11	10.698	1458	1463	1477	rVV	1015271	1366314	64.57%	9.120%
12	11.398	1576	1582	1590	rBV	546214	730734	34.54%	4.878%
13	11.921	1665	1671	1684	rBV	108683	195858	9.26%	1.307%
14	12.639	1790	1793	1798	rVB	24307	30068	1.42%	0.201%
15	12.792	1815	1819	1824	rBV	83175	101064	4.78%	0.675%
16	12.845	1824	1828	1831	rBV	21812	29638	1.40%	0.198%
17	12.980	1845	1851	1861	rBV	1637243	2115919	100.00%	14.124%
18	13.498	1935	1939	1944	rBV	54276	68797	3.25%	0.459%
19	13.880	1999	2004	2022	rBV	60518	129668	6.13%	0.866%
20	14.045	2027	2032	2044	rVB	376962	535114	25.29%	3.572%
21	14.510	2106	2111	2115	rBV3	15583	23771	1.12%	0.159%
22	14.809	2157	2162	2168	rBV3	46510	79444	3.75%	0.530%
23	14.874	2169	2173	2180	rVB2	17309	37725	1.78%	0.252%
24	15.545	2281	2287	2303	rVB	293391	482841	22.82%	3.223%

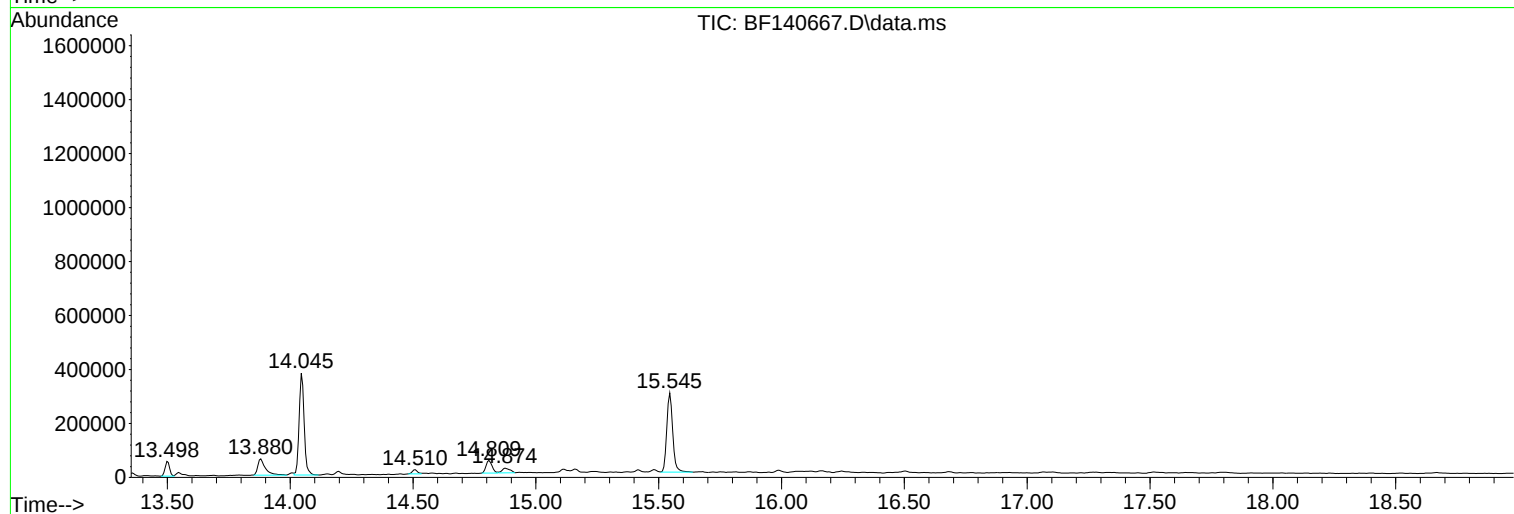
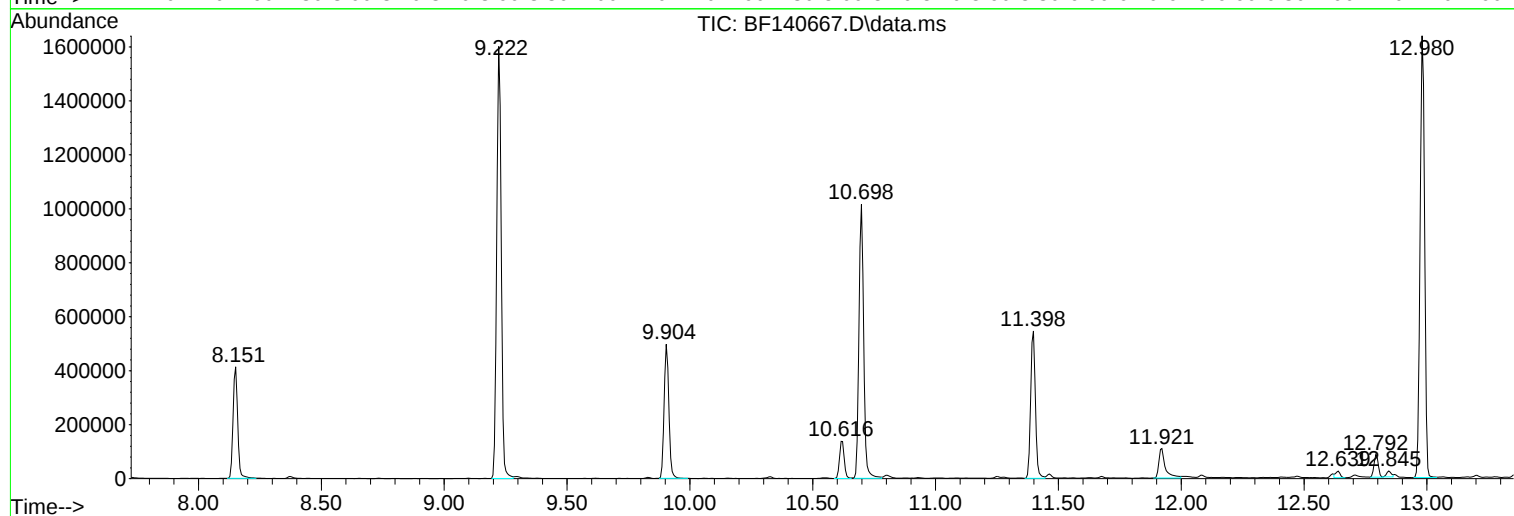
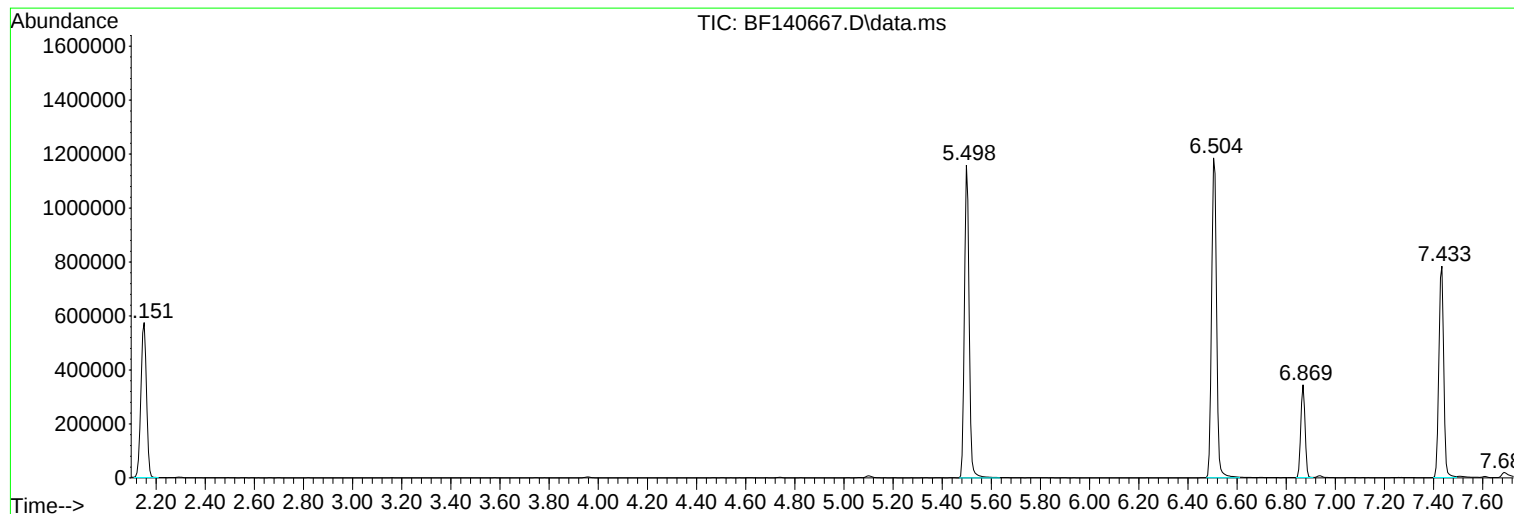
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ClientSampleId :
MH-756-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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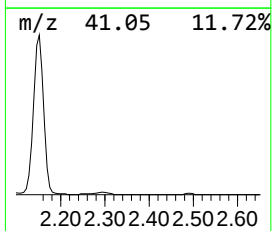
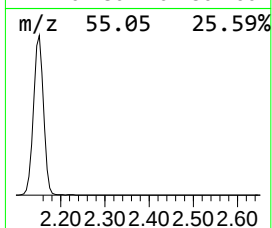
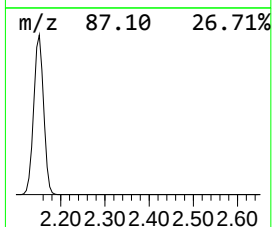
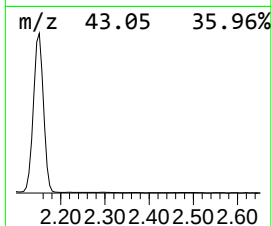
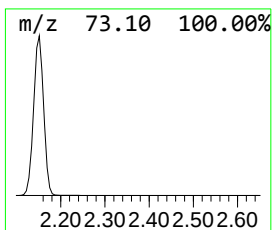
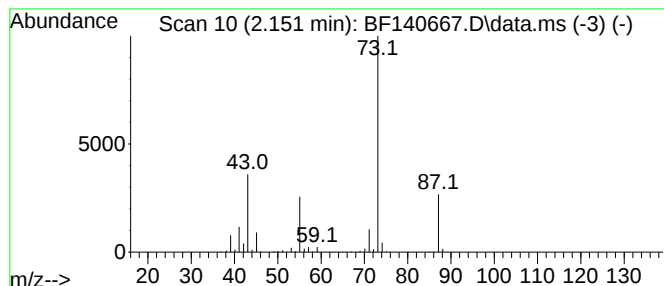
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.151	43.46 ng	906766	1,4-Dichlorobenzene-d4	6.869

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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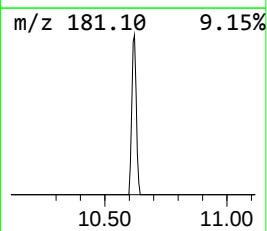
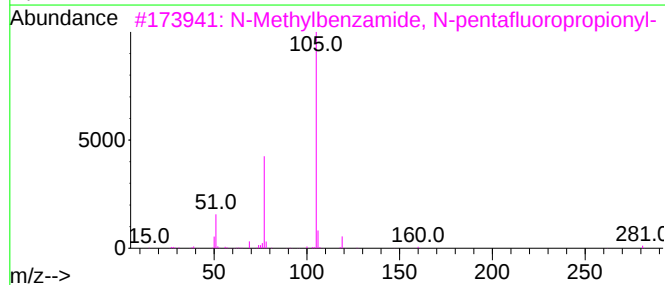
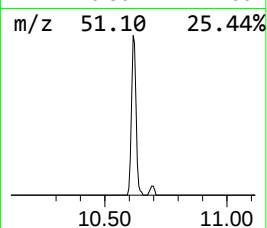
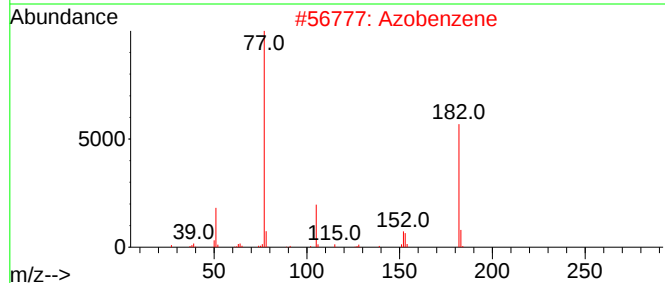
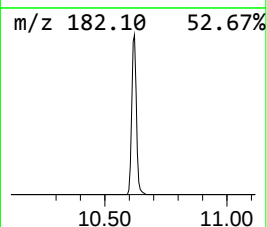
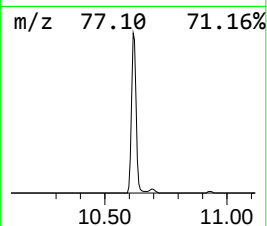
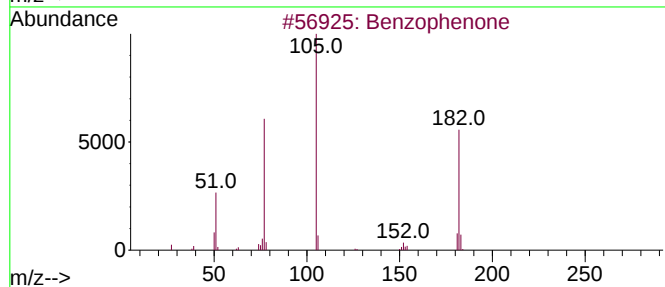
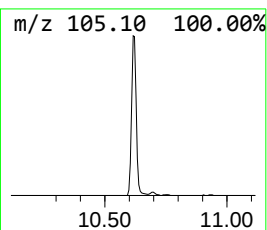
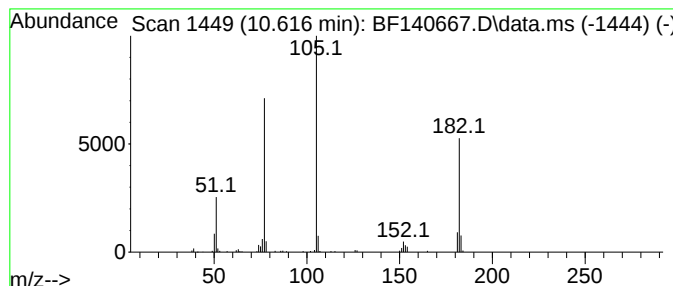
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	5.63 ng	183291	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	59
3			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47



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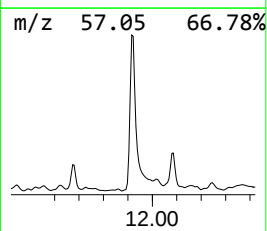
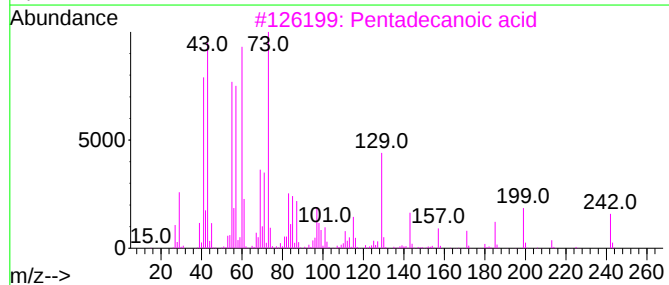
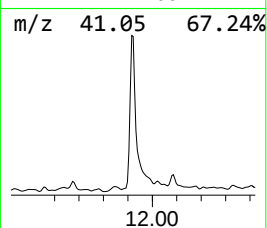
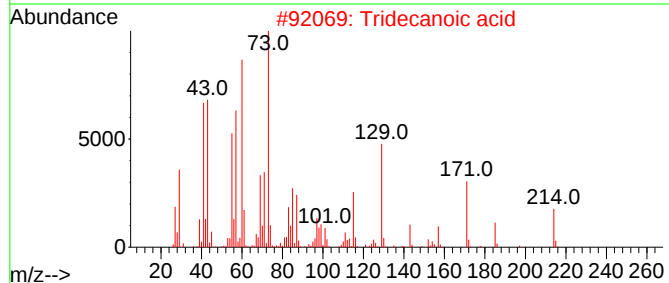
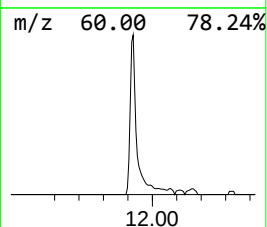
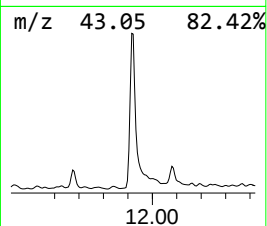
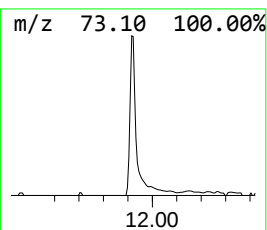
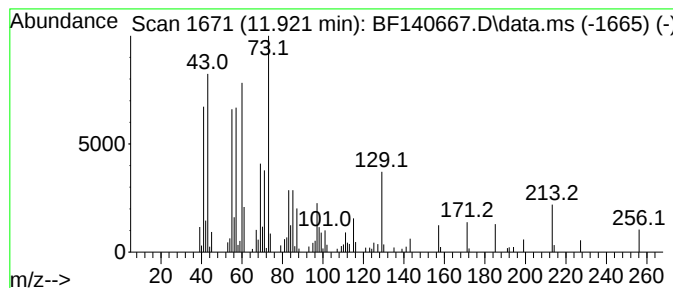
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.921	5.36 ng	195858	Phenanthrene-d10	11.398

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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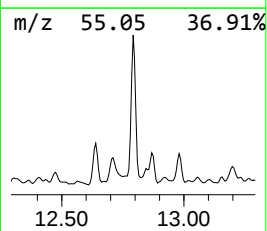
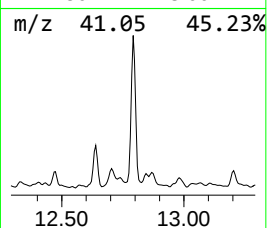
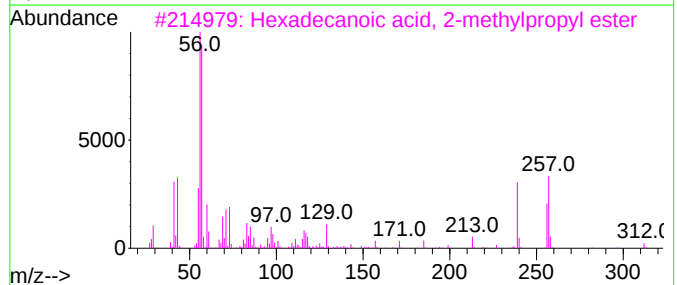
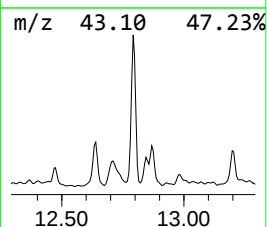
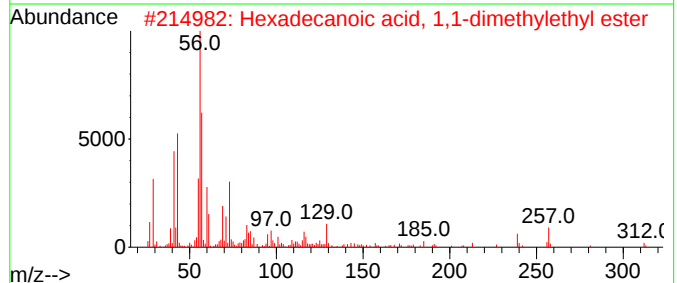
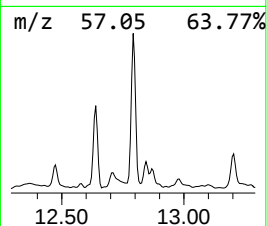
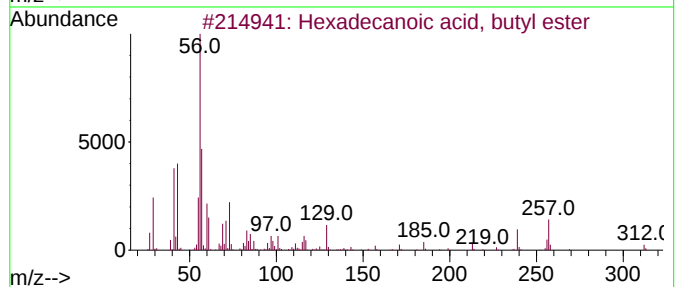
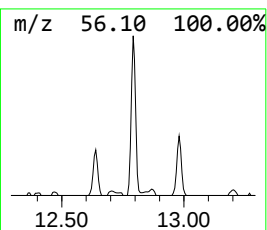
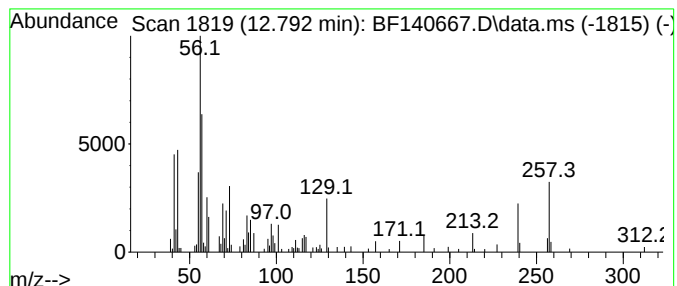
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.792	3.78 ng	101064	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	98
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	95
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	93
4			Nipecotic acid	129	C6H11NO2	000498-95-3	47
5			Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	35



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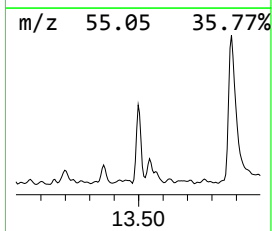
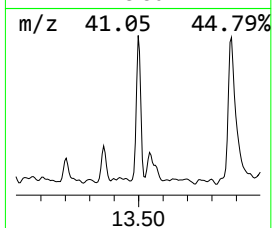
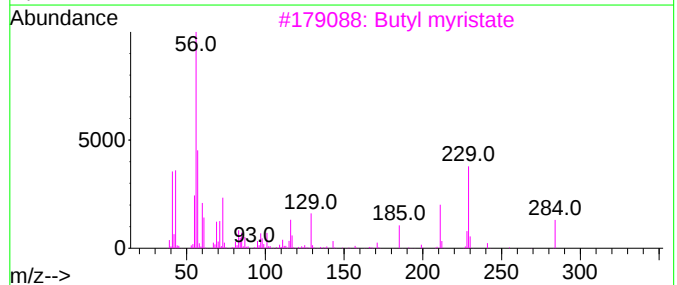
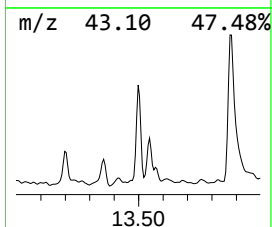
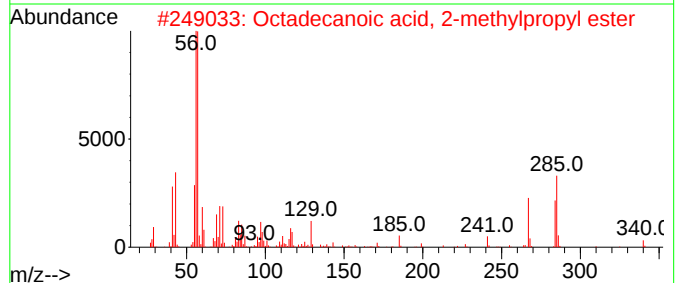
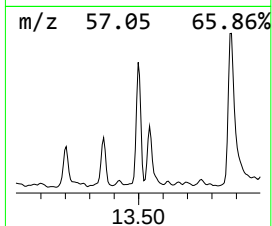
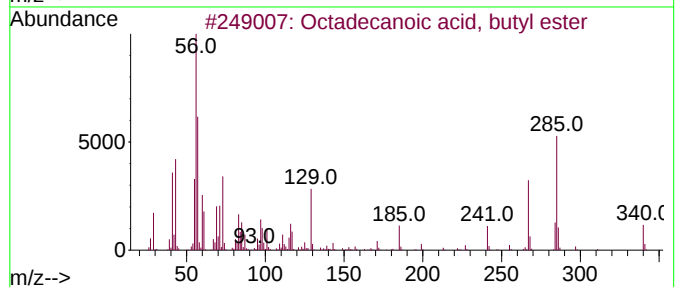
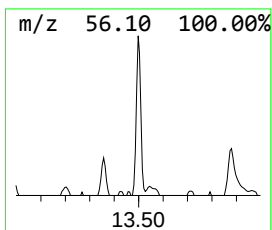
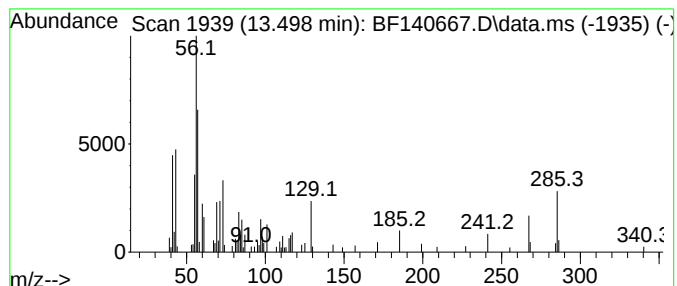
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.498	2.57 ng	68797	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	95
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	70
3	Butyl myristate	284	C18H36O2	000110-36-1	53
4	Nipecotic acid	129	C6H11NO2	000498-95-3	47
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	27



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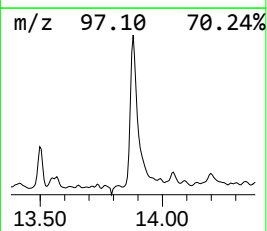
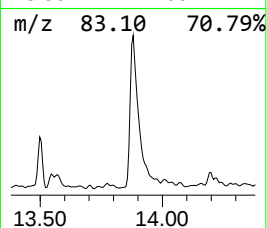
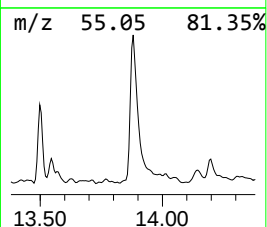
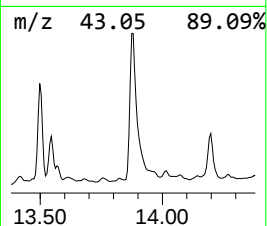
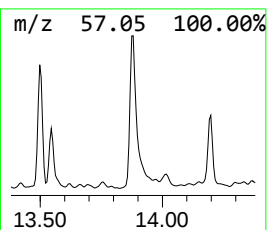
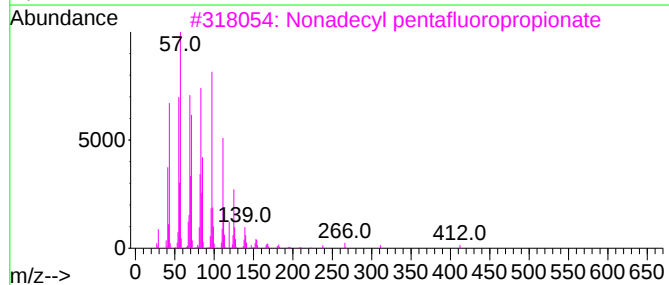
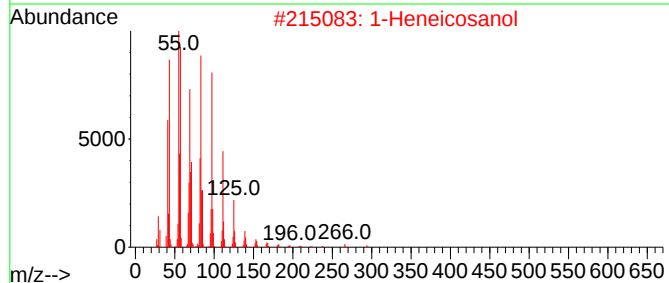
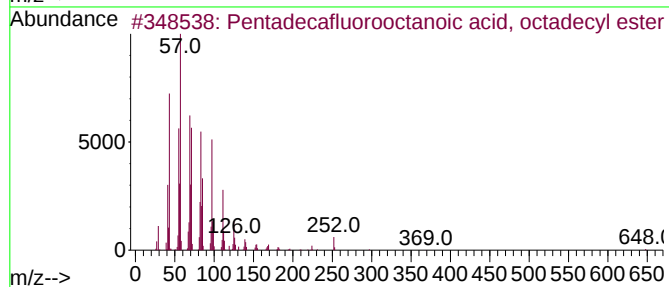
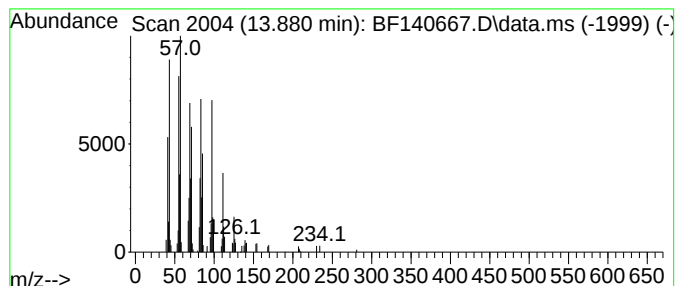
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	4.85 ng	129668	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112724\
Data File : BF140667.D
Acq On : 27 Nov 2024 14:04
Operator : RC/JU
Sample : P4985-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-756-WC

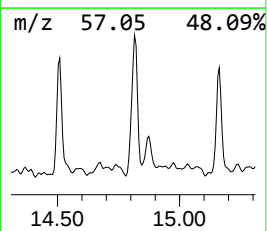
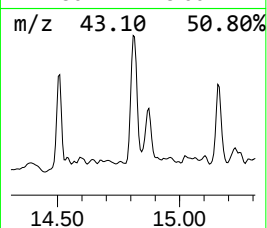
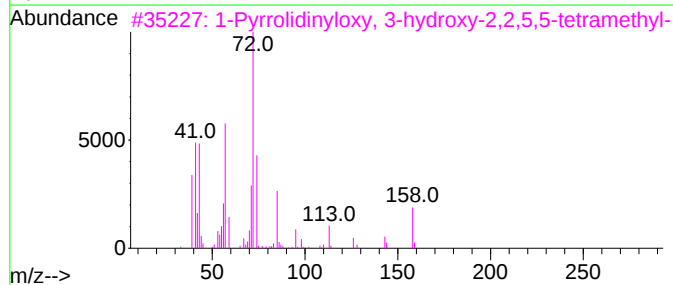
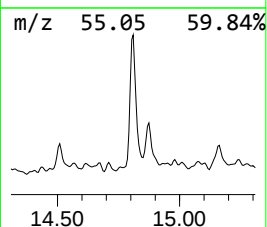
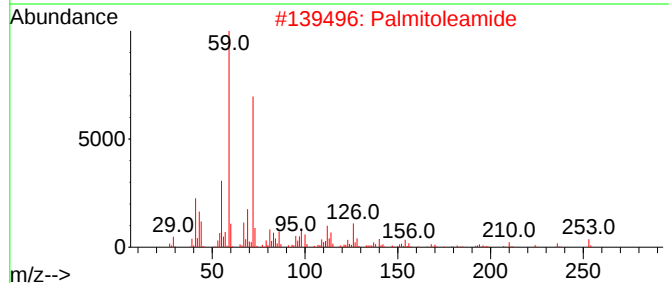
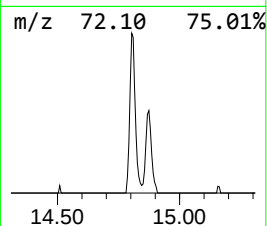
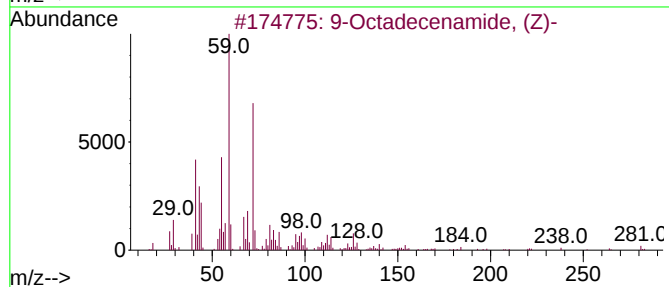
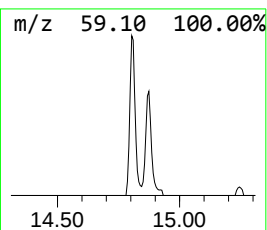
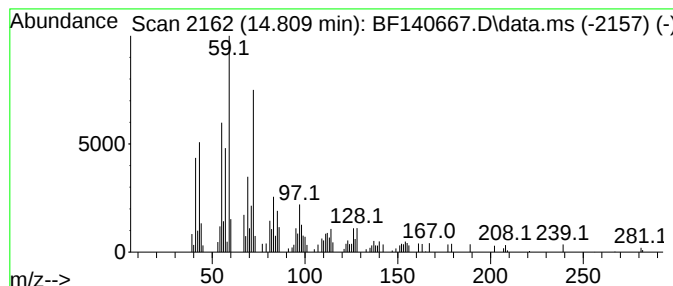
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	3.29 ng	79444	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2			Palmitoleamide	253	C16H31NO	106010-22-4	64
3			1-Pyrrolidinyloxy, 3-hydroxy-2,2...	158	C8H16NO2	002154-37-2	35
4			Butanal, 2-ethyl-3-methyl-	114	C7H14O	026254-92-2	25
5			Isobutyl-propyl-amine	115	C7H17N	039190-66-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112724\
Data File : BF140667.D
Acq On : 27 Nov 2024 14:04
Operator : RC/JU
Sample : P4985-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-756-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.151	43.5	ng	906766	1	6.869	417295	20.0
Benzophenone	10.616	5.6	ng	183291	3	9.904	651108	20.0
n-Hexadecanoic ...	11.921	5.4	ng	195858	4	11.398	730734	20.0
Hexadecanoic ac...	12.792	3.8	ng	101064	5	14.045	535114	20.0
Octadecanoic ac...	13.498	2.6	ng	68797	5	14.045	535114	20.0
Pentadecafluoro...	13.880	4.8	ng	129668	5	14.045	535114	20.0
9-Octadecenamid...	14.810	3.3	ng	79444	6	15.545	482841	20.0