

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
 Data File : BF140171.D
 Acq On : 30 Oct 2024 21:17
 Operator : RC/JU
 Sample : P4594-09
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BP-F16

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140171.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	5	12	29	rVB	743367	1183745	80.65%	9.695%
2	5.504	574	580	585	rBV	1126849	1467715	100.00%	12.020%
3	6.504	744	750	762	rVB	1110090	1464663	99.79%	11.995%
4	6.887	810	815	820	rBV	399377	491221	33.47%	4.023%
5	7.440	904	909	914	rBV	649093	819909	55.86%	6.715%
6	7.692	948	952	958	rBV	38012	45909	3.13%	0.376%
7	8.163	1027	1032	1043	rVB	460624	565358	38.52%	4.630%
8	8.375	1064	1068	1076	rVB	12475	15595	1.06%	0.128%
9	9.239	1210	1215	1220	rBV	953477	1161932	79.17%	9.516%
10	9.922	1326	1331	1338	rVB	418943	534485	36.42%	4.377%
11	10.639	1448	1453	1460	rBV	76127	92744	6.32%	0.760%
12	10.716	1460	1466	1478	rBV	666964	841920	57.36%	6.895%
13	11.416	1580	1585	1591	rBV	449760	564694	38.47%	4.625%
14	11.945	1670	1675	1687	rBV	164992	278676	18.99%	2.282%
15	12.674	1797	1799	1805	rVB	17637	19508	1.33%	0.160%
16	12.733	1805	1809	1816	rBV2	35209	64726	4.41%	0.530%
17	12.827	1821	1825	1829	rVV	58795	74954	5.11%	0.614%
18	13.010	1851	1856	1865	rBV	1083574	1395976	95.11%	11.433%
19	13.539	1943	1946	1950	rBV	40977	47017	3.20%	0.385%
20	13.916	2006	2010	2020	rBV	77115	132649	9.04%	1.086%
21	14.068	2031	2036	2045	rBV	441752	595603	40.58%	4.878%
22	15.568	2287	2291	2297	rBV	220784	351159	23.93%	2.876%

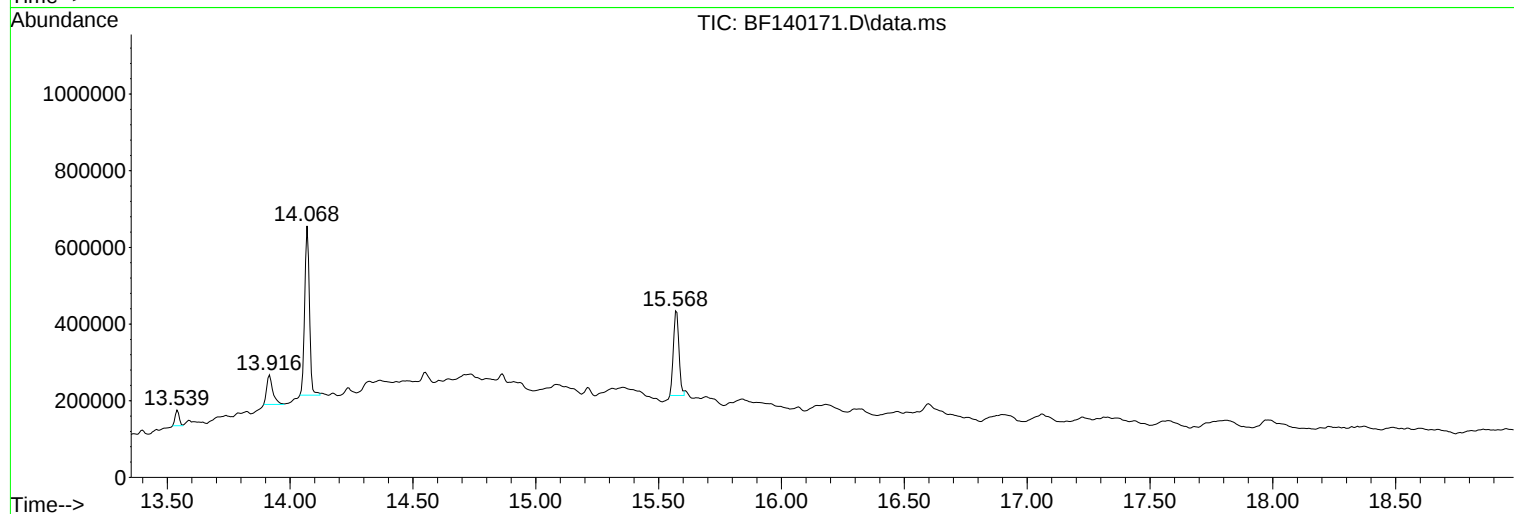
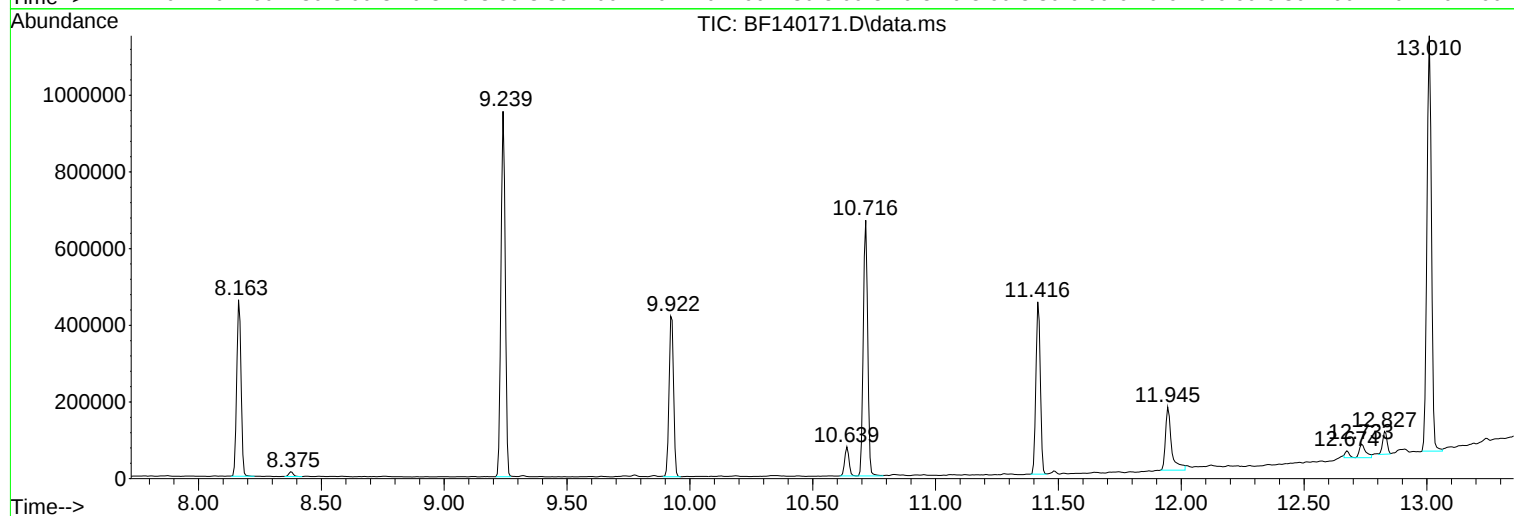
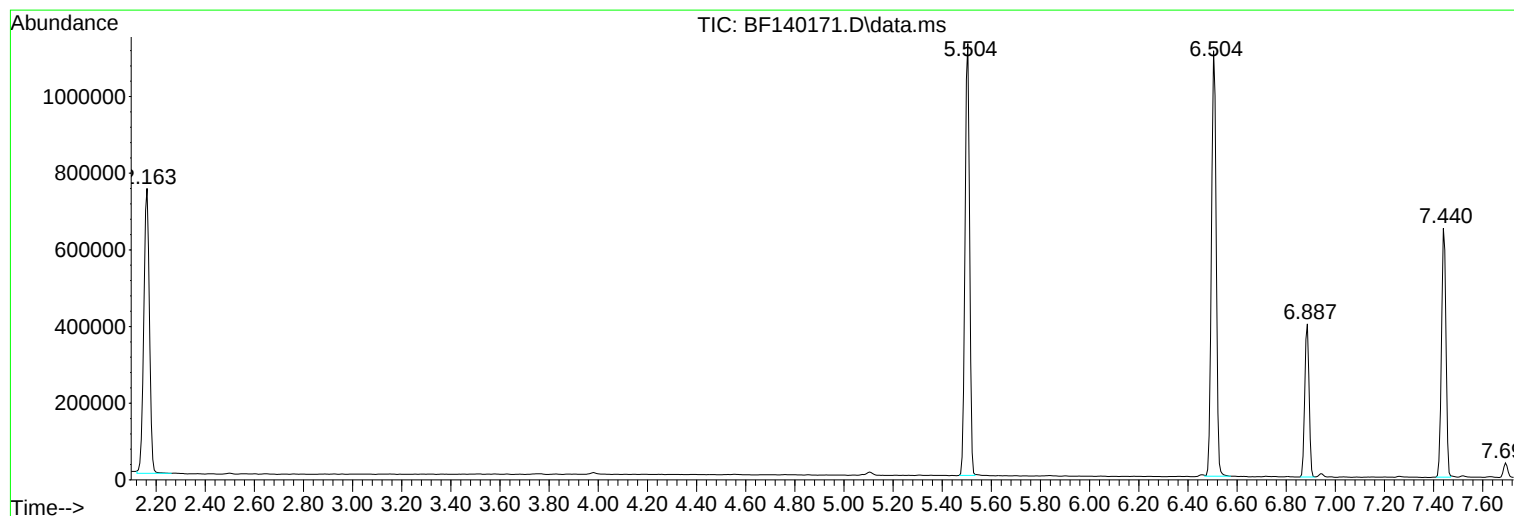
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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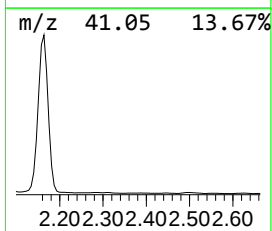
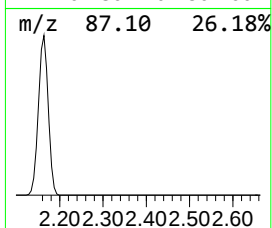
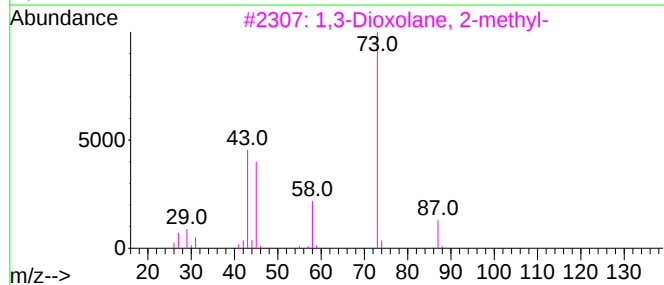
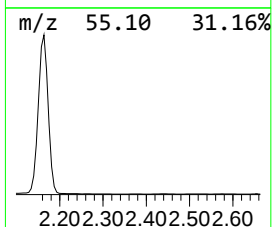
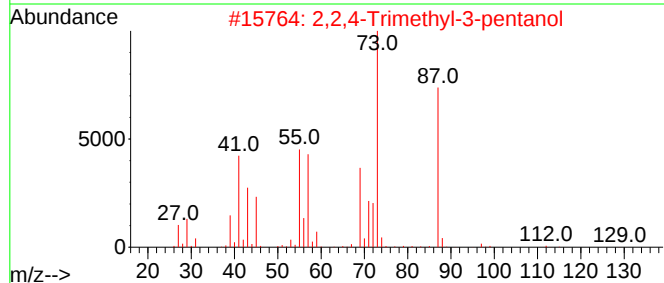
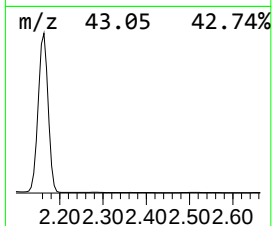
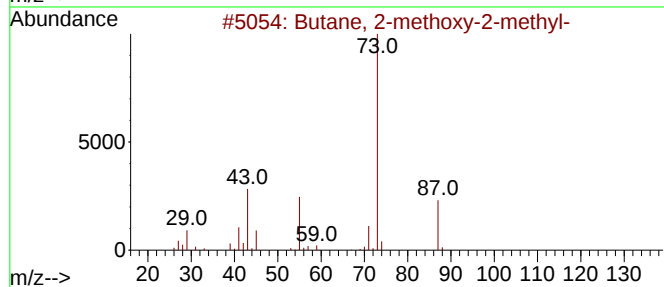
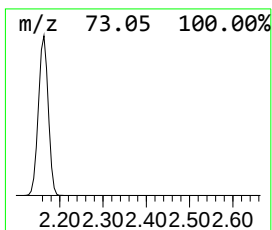
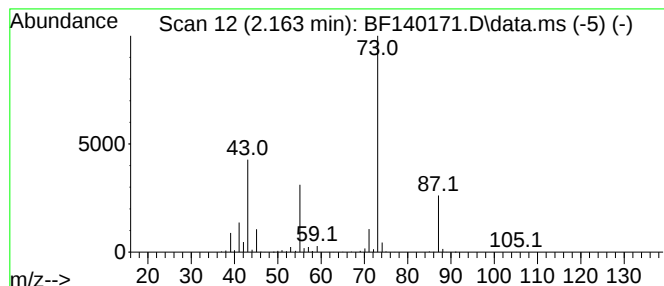
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.163	48.20 ng	1183750	1,4-Dichlorobenzene-d4	6.887

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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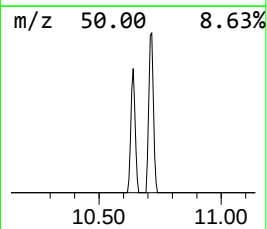
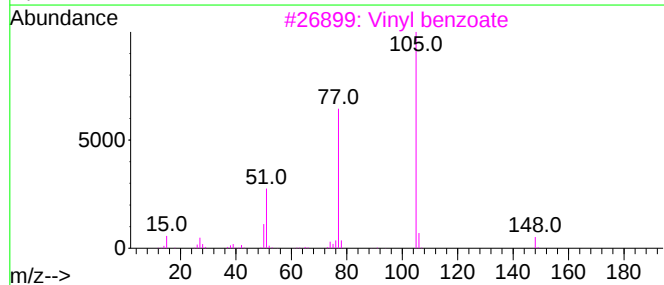
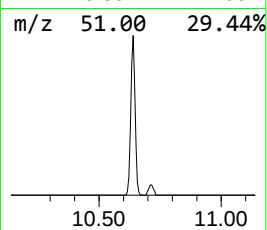
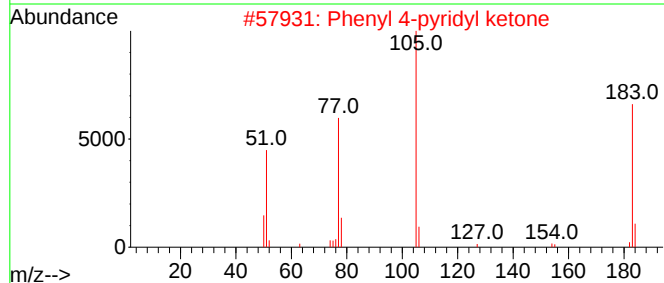
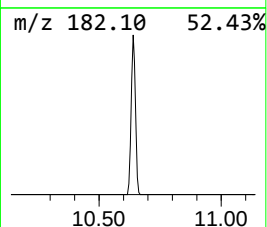
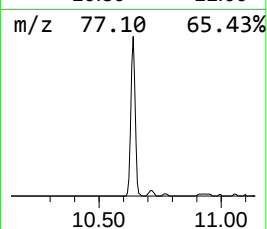
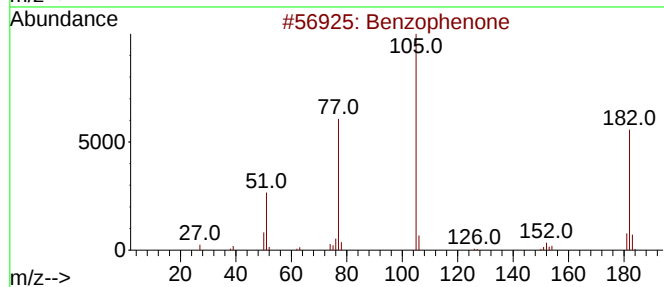
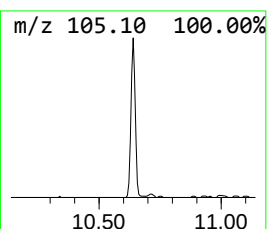
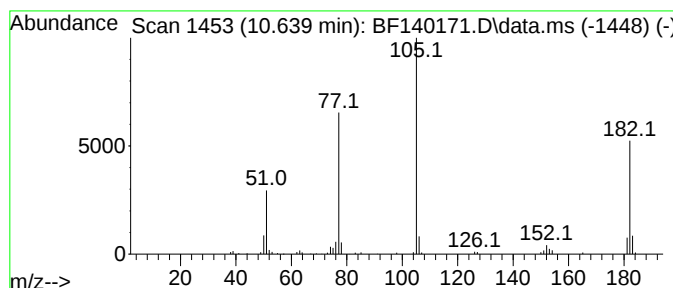
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	3.47 ng	92744	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			Vinyl benzoate	148	C9H8O2	000769-78-8	47
4			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	47
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47



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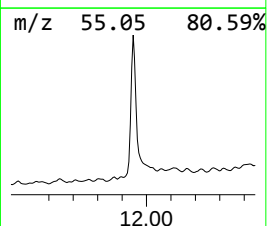
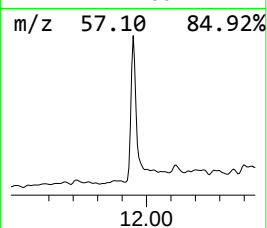
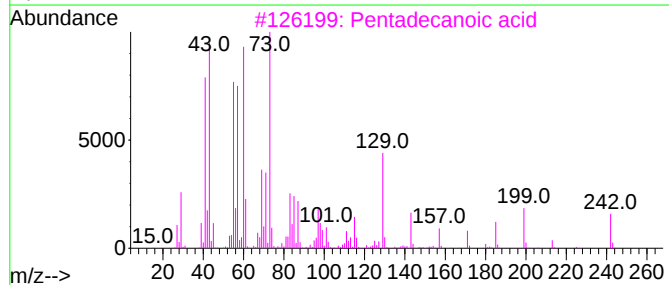
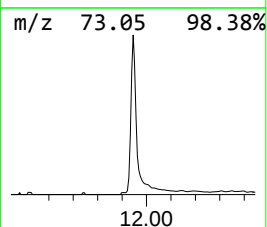
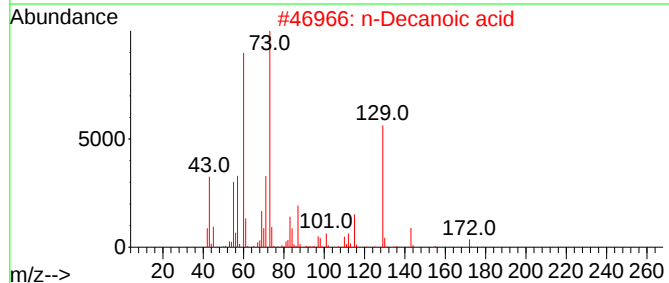
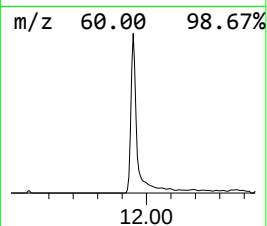
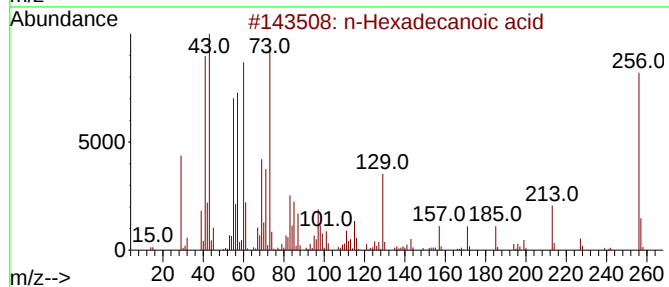
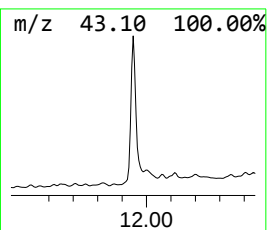
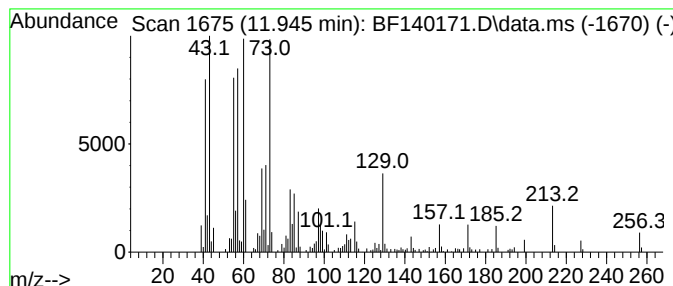
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	9.87 ng	278676	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	90
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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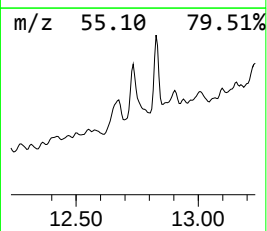
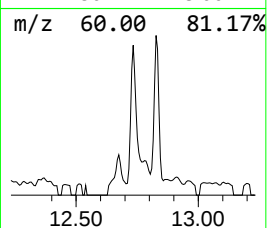
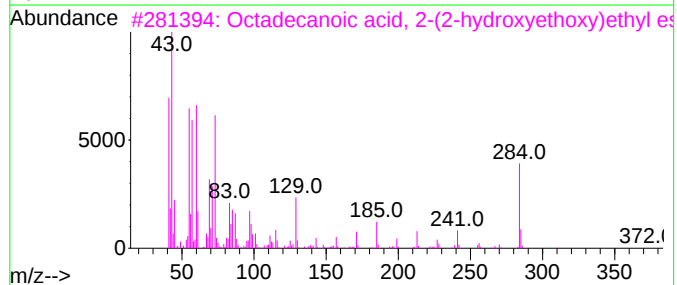
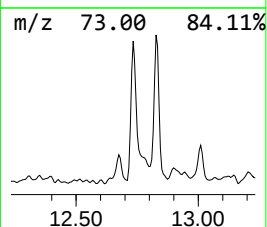
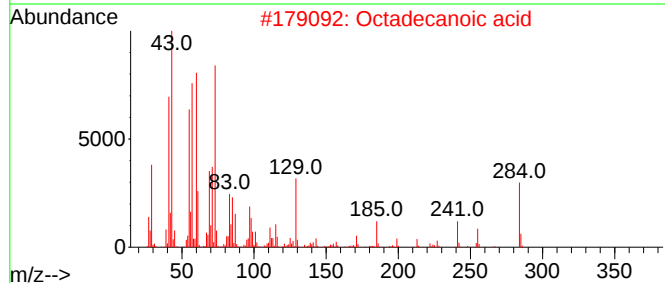
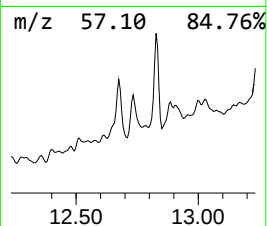
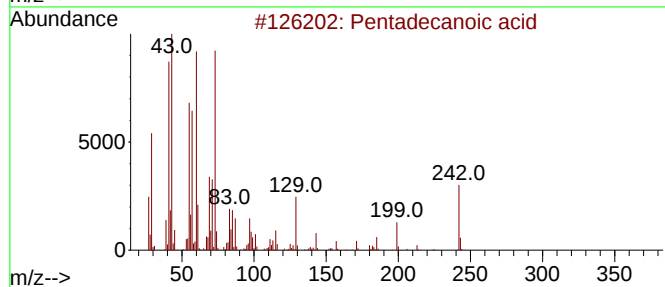
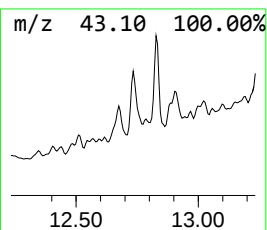
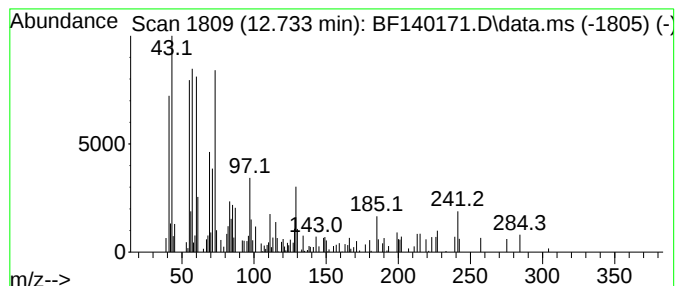
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	2.29 ng	64726	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
2			Octadecanoic acid	284	C18H36O2	000057-11-4	94
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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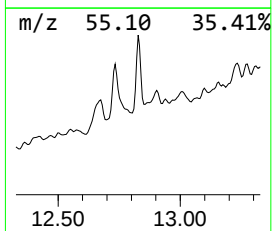
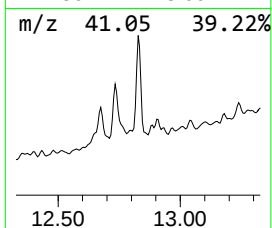
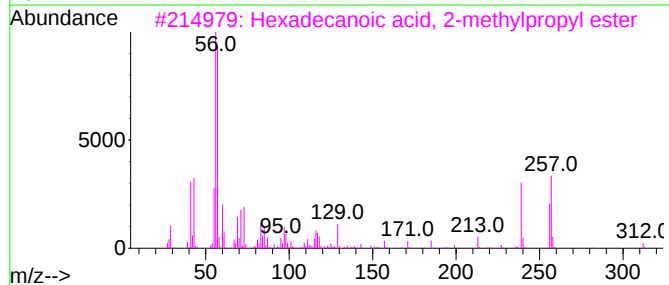
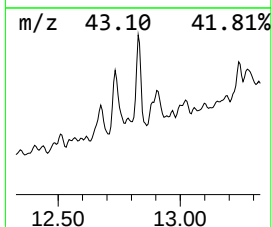
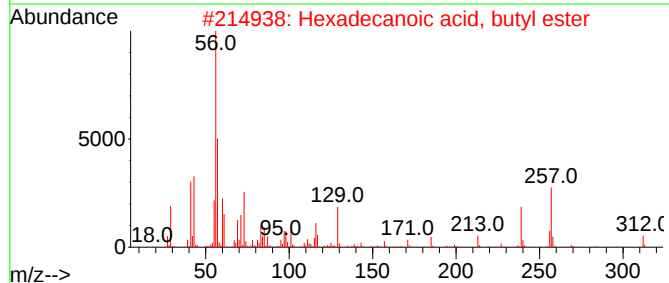
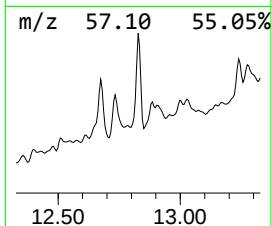
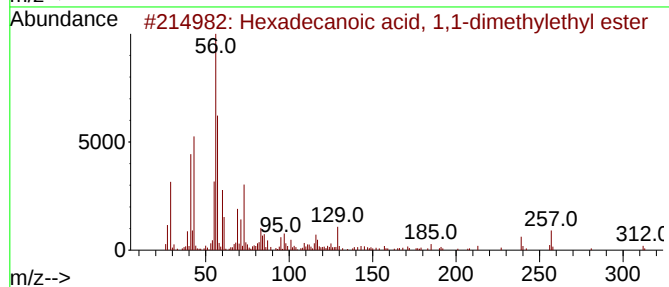
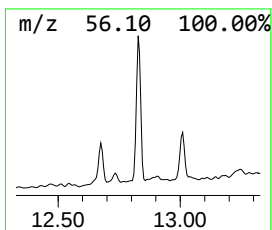
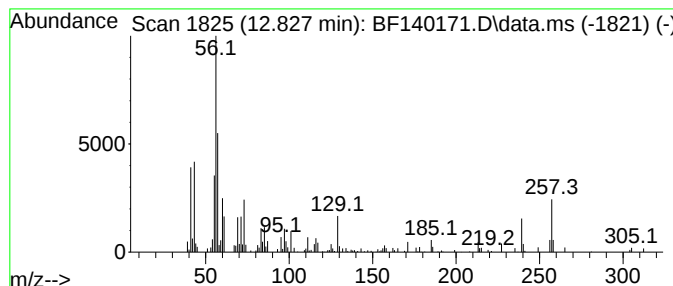
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.827	2.52 ng	74954	Chrysene-d12	14.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	78
4			1-[N-Aziridyl]heptene-3	139	C9H17N	1000255-07-6	35
5			Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	30



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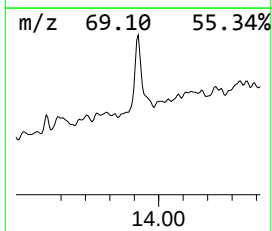
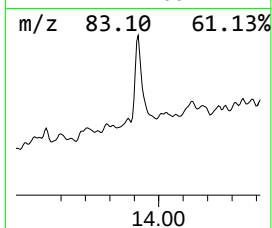
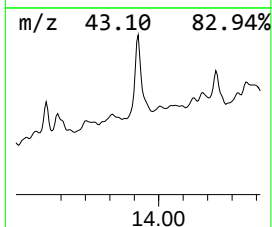
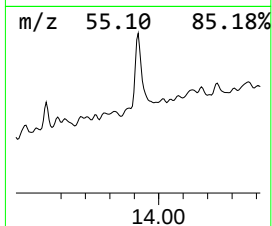
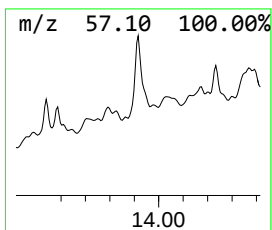
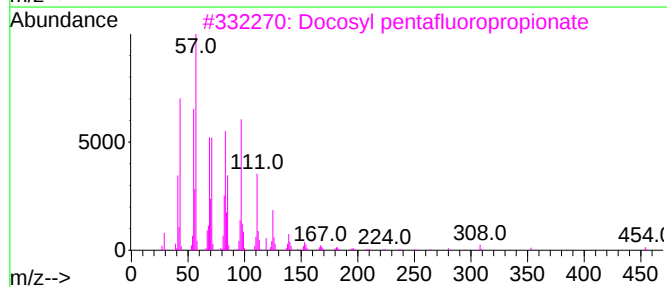
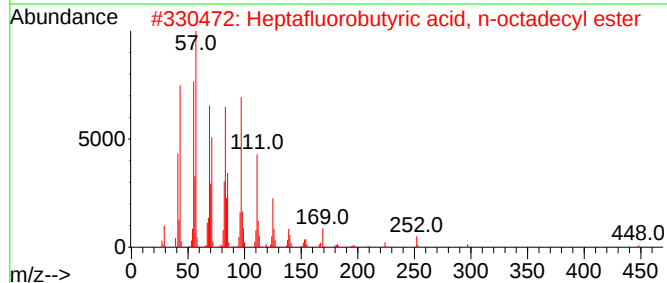
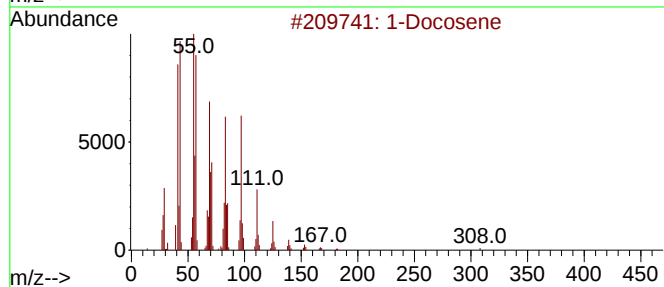
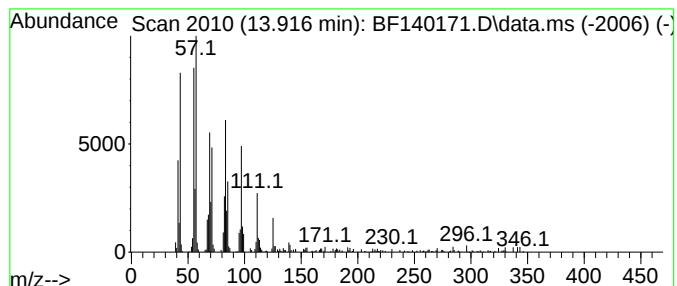
Instrument :
BNA_F
ClientSampleId :
BP-F16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.916	4.45 ng	132649	Chrysene-d12	14.069	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	96
2	Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140171.D
Acq On : 30 Oct 2024 21:17
Operator : RC/JU
Sample : P4594-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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	48.2	ng	1183750	1	6.887	491221	20.0
Benzophenone	10.639	3.5	ng	92744	3	9.922	534485	20.0
n-Hexadecanoic ...	11.945	9.9	ng	278676	4	11.416	564694	20.0
Pentadecanoic acid	12.733	2.3	ng	64726	4	11.416	564694	20.0
Hexadecanoic ac...	12.827	2.5	ng	74954	5	14.069	595603	20.0
1-Docosene	13.916	4.5	ng	132649	5	14.069	595603	20.0