

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
 Data File : BF140017.D
 Acq On : 24 Oct 2024 22:58
 Operator : RC/JU
 Sample : P4487-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BP-B5

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: BF140017.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	7	15	22	rBV	430823	676053	34.04%	4.555%
2	5.110	505	513	521	rVB2	15545	25300	1.27%	0.170%
3	5.504	574	580	585	rBV	1304230	1710898	86.14%	11.528%
4	5.628	596	601	608	rVB	18157	28331	1.43%	0.191%
5	5.992	658	663	670	rBV	61467	89066	4.48%	0.600%
6	6.122	678	685	693	rVB4	14220	30660	1.54%	0.207%
7	6.269	706	710	711	rBV	30434	34469	1.74%	0.232%
8	6.287	711	713	718	rVB	37339	46183	2.33%	0.311%
9	6.504	744	750	756	rVV	1236434	1721912	86.69%	11.602%
10	6.887	810	815	820	rBV	396395	484092	24.37%	3.262%
11	7.445	904	910	915	rBV	896017	1146943	57.74%	7.728%
12	7.698	948	953	958	rBV	59608	69247	3.49%	0.467%
13	8.169	1027	1033	1038	rBV	506267	621923	31.31%	4.191%
14	8.381	1063	1069	1076	rVB2	26240	36859	1.86%	0.248%
15	9.245	1210	1216	1226	rBV	1540860	1986244	100.00%	13.383%
16	9.922	1326	1331	1341	rBV	521266	655489	33.00%	4.417%
17	10.633	1447	1452	1459	rBV	393149	502537	25.30%	3.386%
18	10.710	1459	1465	1480	rVV	881883	1115493	56.16%	7.516%
19	10.827	1480	1485	1491	rVB2	12109	20451	1.03%	0.138%
20	10.945	1501	1505	1511	rVB	53098	63823	3.21%	0.430%
21	11.410	1579	1584	1589	rBV	457985	566983	28.55%	3.820%
22	11.933	1668	1673	1688	rBV	231474	348248	17.53%	2.347%
23	12.433	1753	1758	1760	rBV	14121	20315	1.02%	0.137%
24	12.639	1788	1793	1802	rVB9	8535	25243	1.27%	0.170%
25	12.716	1802	1806	1814	rBV	42525	74457	3.75%	0.502%
26	12.992	1848	1853	1861	rBV	1011392	1282979	64.59%	8.645%
27	13.227	1887	1893	1897	rBV	18393	31660	1.59%	0.213%
28	13.568	1947	1951	1962	rVB	20719	38398	1.93%	0.259%
29	13.892	2002	2006	2016	rBV	75499	146296	7.37%	0.986%
30	14.045	2027	2032	2039	rBV	297396	391858	19.73%	2.640%
31	14.210	2057	2060	2070	rVB	20446	32743	1.65%	0.221%
32	14.515	2109	2112	2125	rBV3	18664	33432	1.68%	0.225%
33	14.810	2157	2162	2171	rBV2	97258	188300	9.48%	1.269%
34	14.904	2174	2178	2184	rVB	40643	59284	2.98%	0.399%
35	15.168	2220	2223	2234	rVB3	17402	28240	1.42%	0.190%
36	15.527	2278	2284	2298	rVB	300566	506693	25.51%	3.414%

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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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

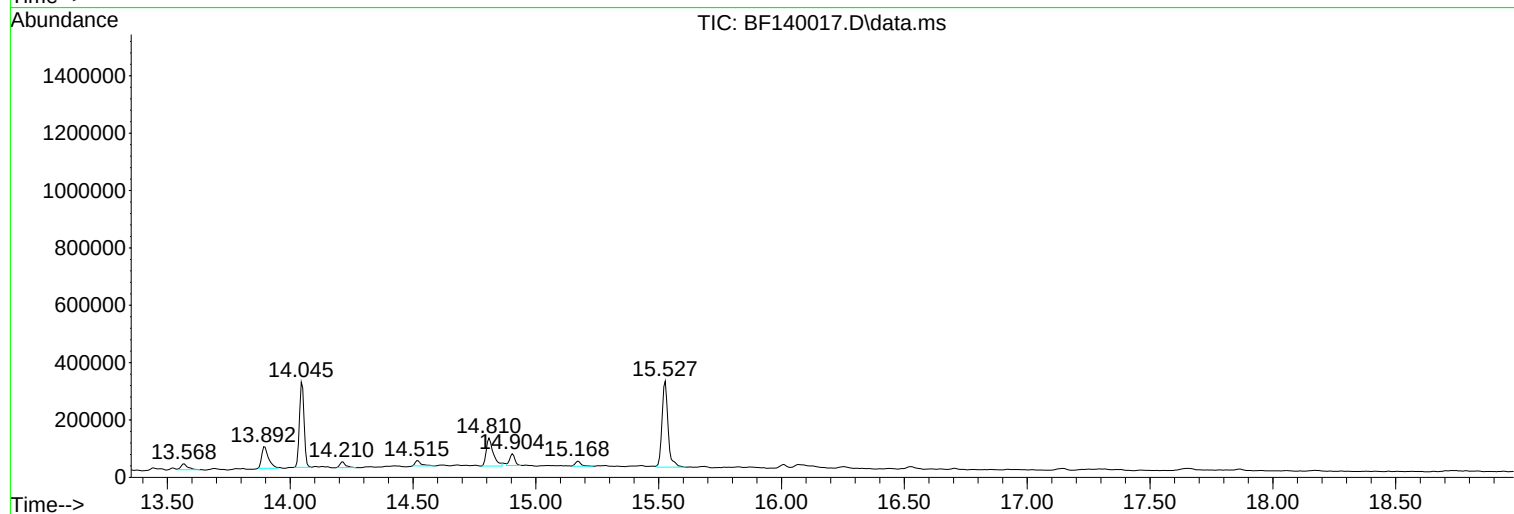
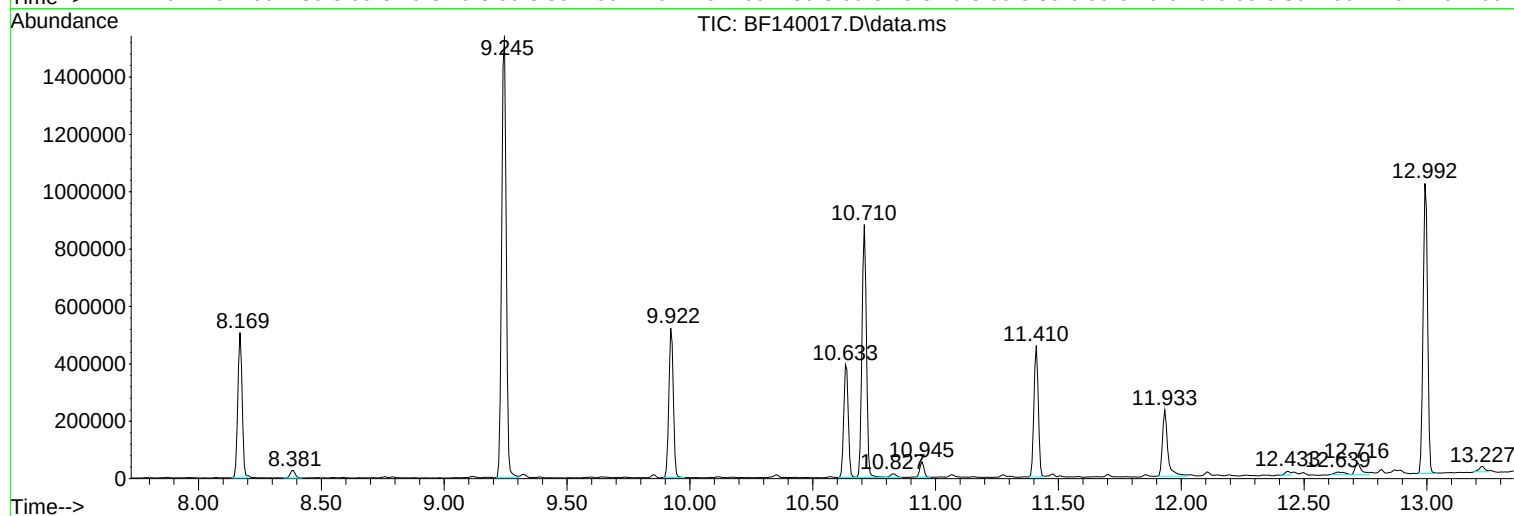
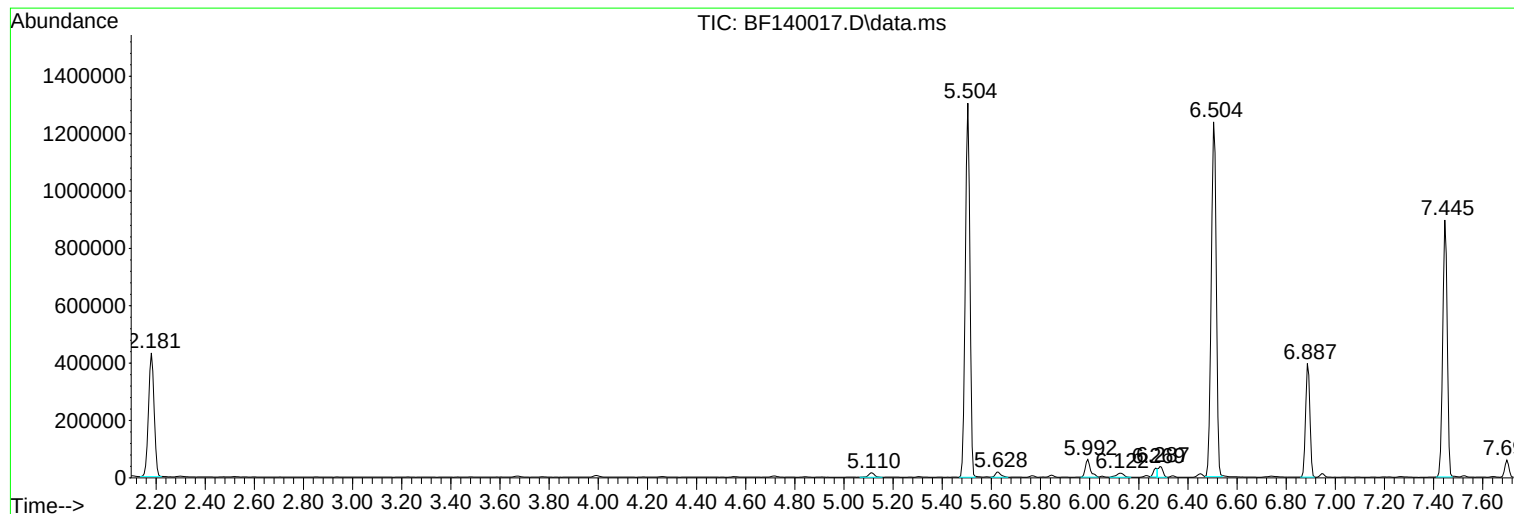
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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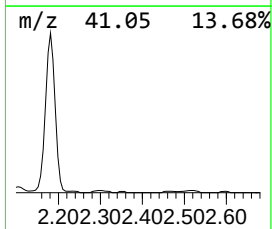
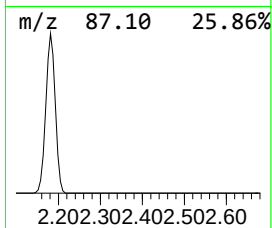
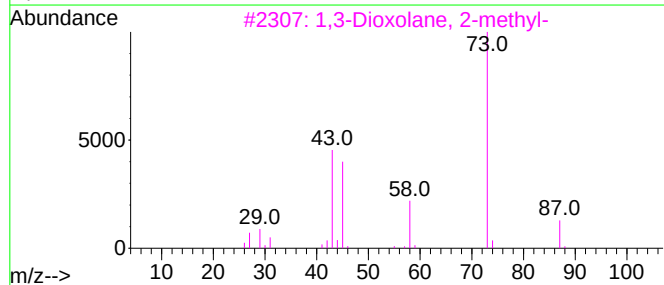
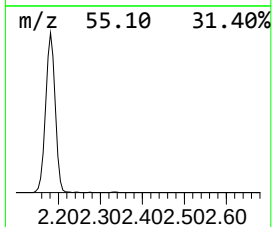
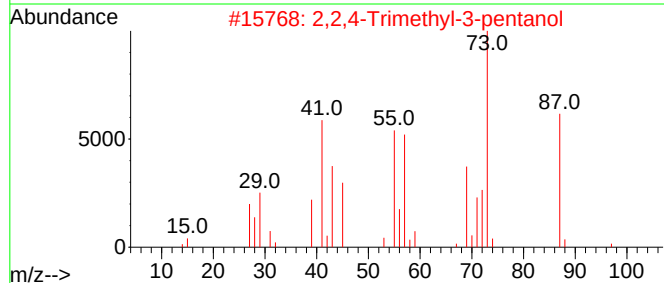
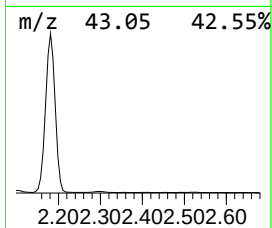
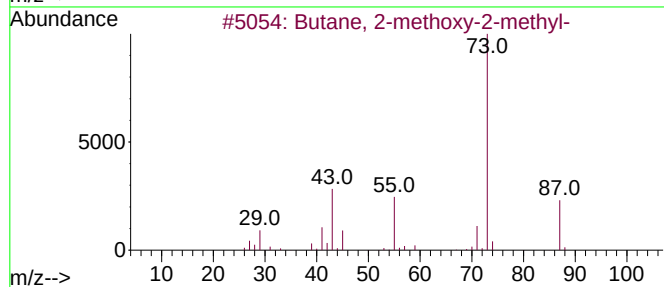
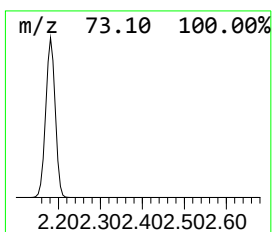
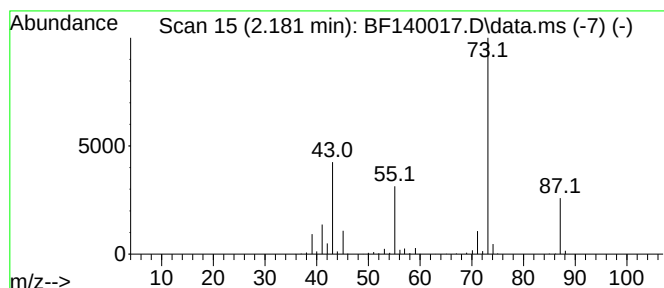
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.181	27.93 ng	676053	1,4-Dichlorobenzene-d4	6.886

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
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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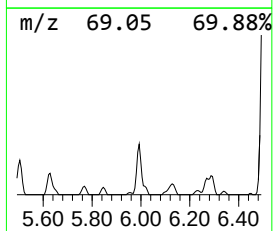
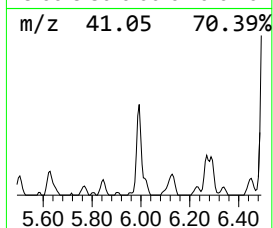
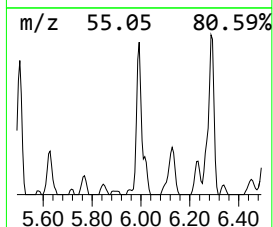
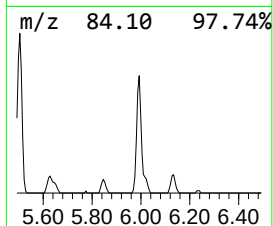
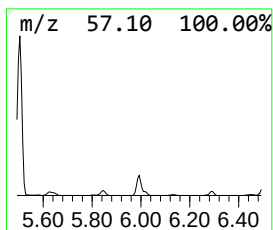
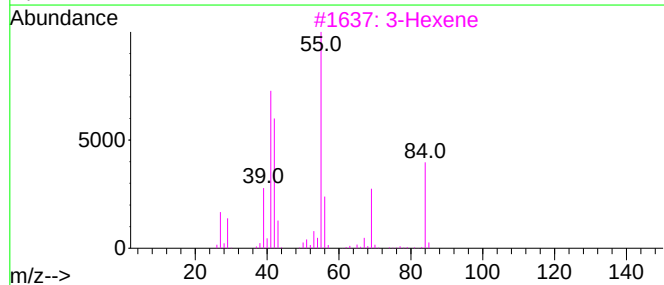
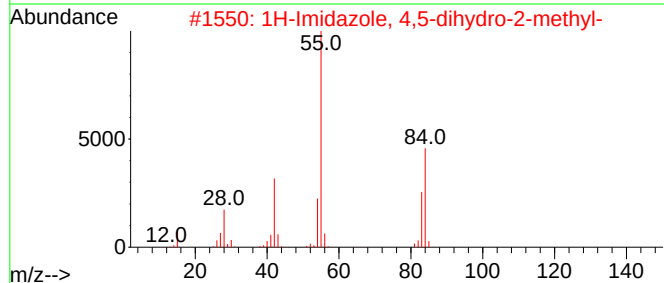
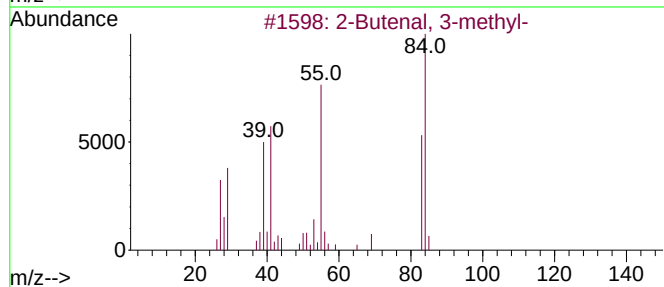
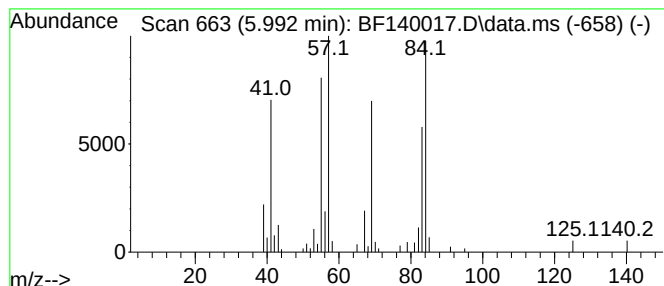
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Butenal, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.992	3.68 ng	89066	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	53
2			1H-Imidazole, 4,5-dihydro-2-methyl-	84	C4H8N2	000534-26-9	47
3			3-Hexene	84	C6H12	000592-47-2	43
4			Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	38
5			2-Pentenal, (E)-	84	C5H8O	001576-87-0	38



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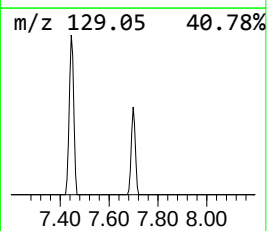
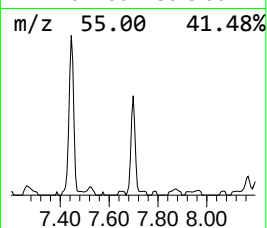
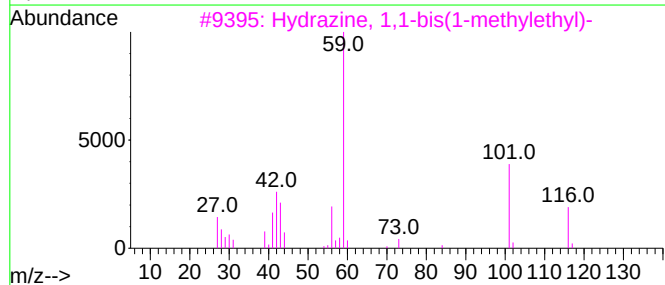
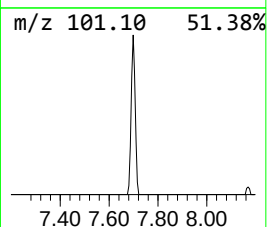
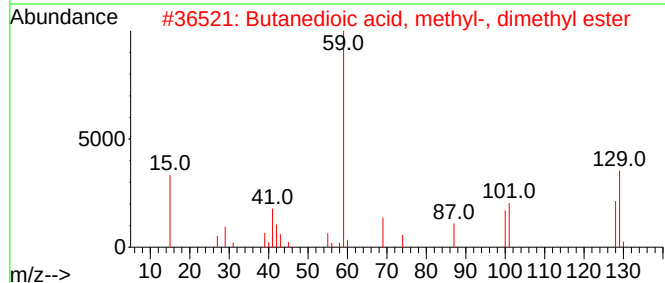
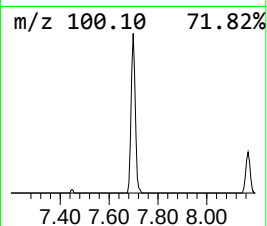
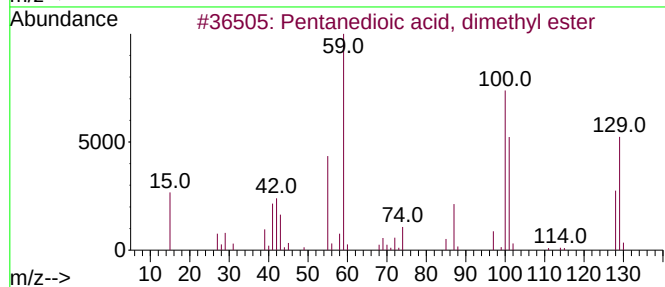
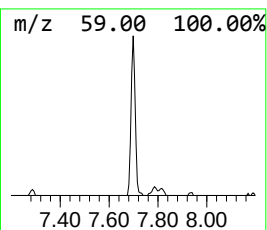
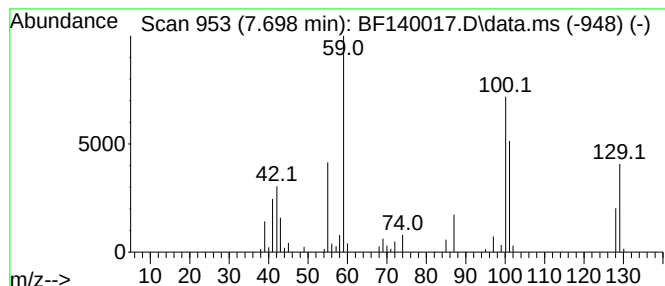
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Pentanedioic acid, dimethyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.698	2.23 ng	69247	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	90
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	42
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	32
4			Hydrazine, trimethyl-	74	C3H10N2	001741-01-1	22
5			Hydrazine, (1-methylethyl)-	74	C3H10N2	002257-52-5	22



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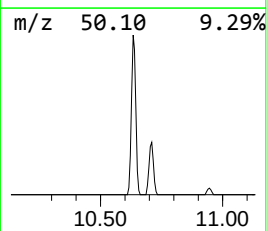
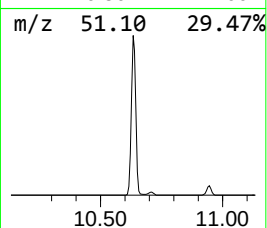
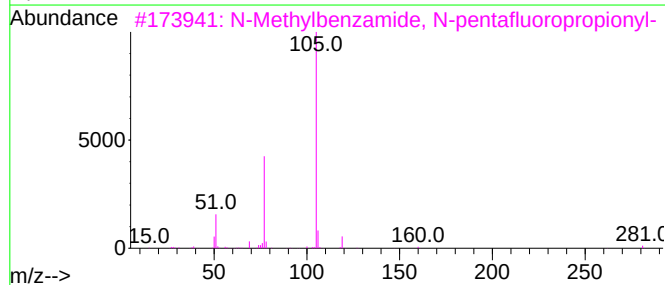
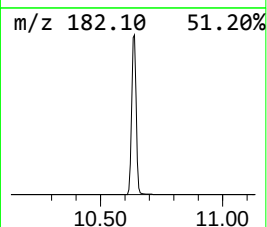
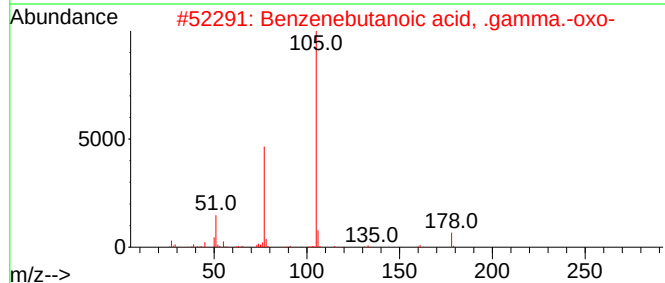
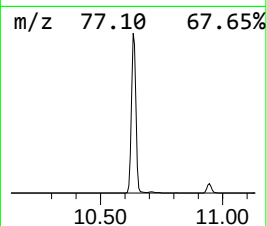
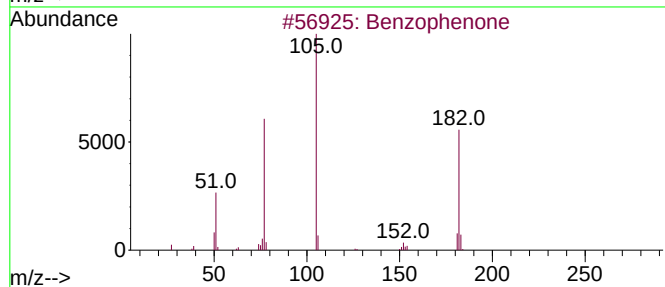
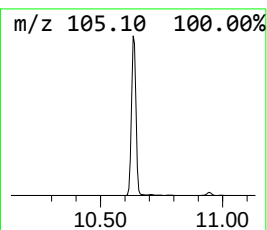
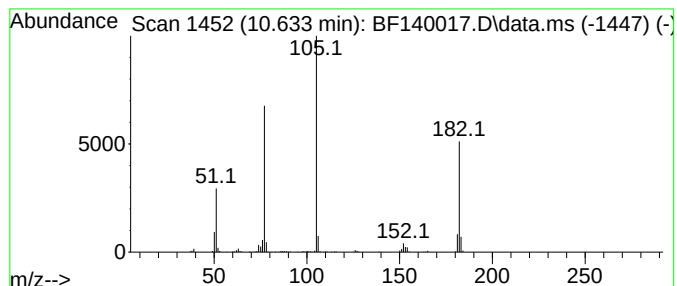
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	15.33 ng	502537	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
3			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
5			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	50



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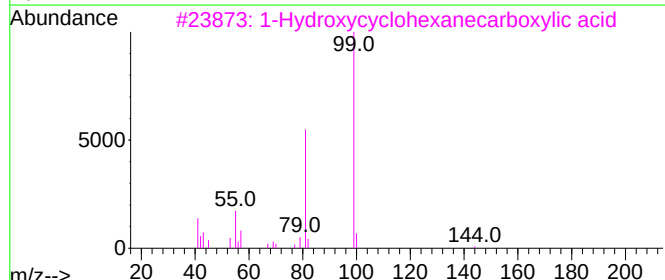
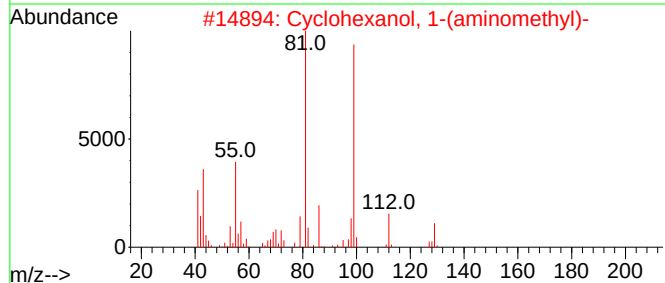
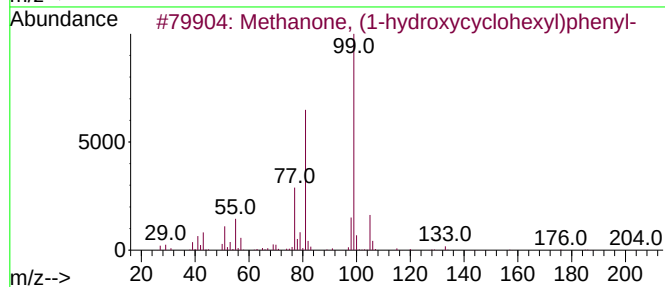
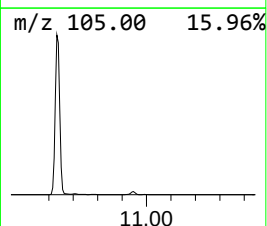
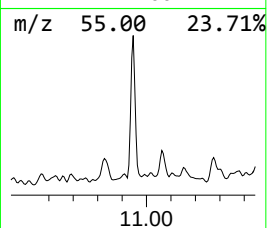
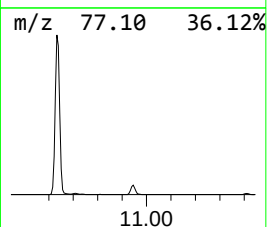
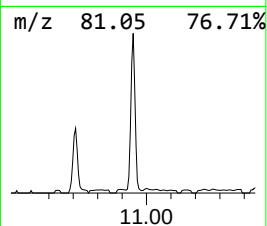
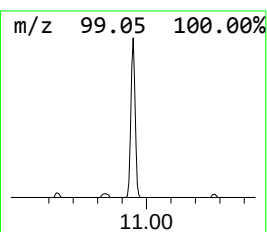
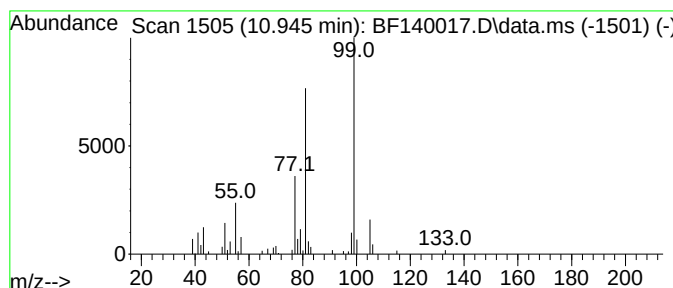
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Methanone, (1-hydroxycyclohexyl) Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.945	2.25 ng	63823	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	50
3			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	45
4			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	45
5			Furan, tetrahydro-2,2-dimethyl-5...	156	C10H20O	033978-70-0	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140017.D
Acq On : 24 Oct 2024 22:58
Operator : RC/JU
Sample : P4487-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-B5

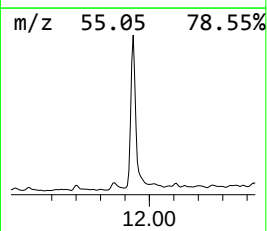
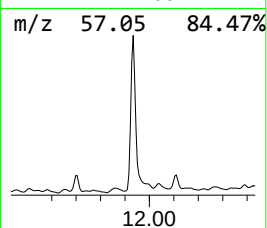
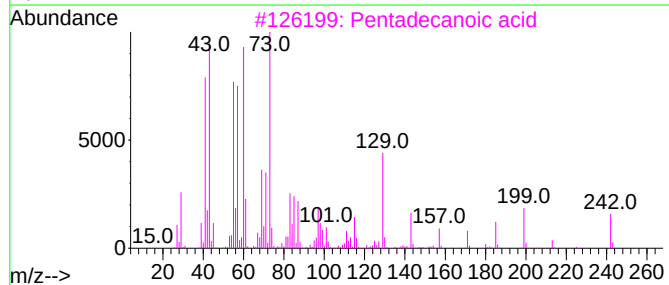
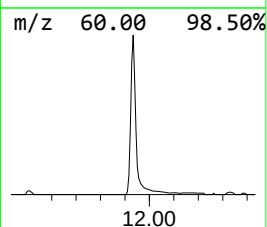
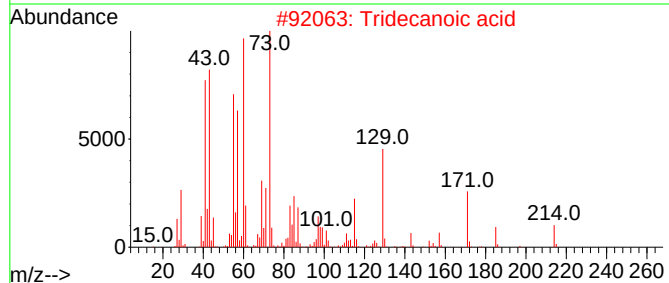
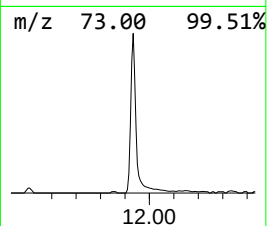
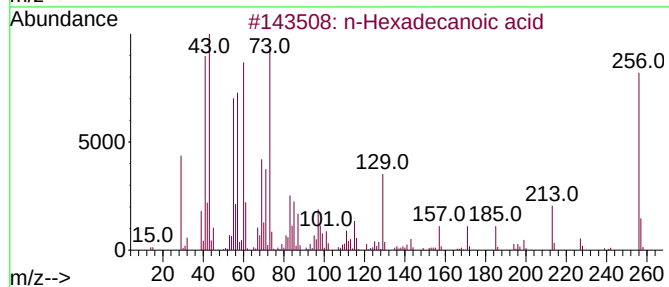
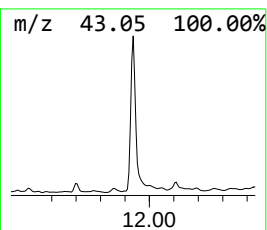
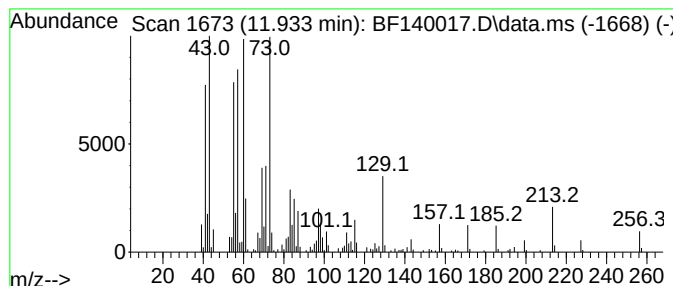
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	12.28 ng	348248	Phenanthrene-d10	11.410

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	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140017.D
Acq On : 24 Oct 2024 22:58
Operator : RC/JU
Sample : P4487-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-B5

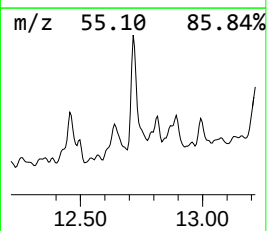
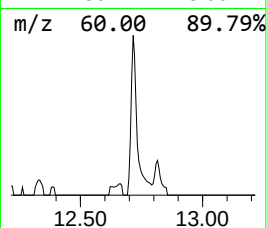
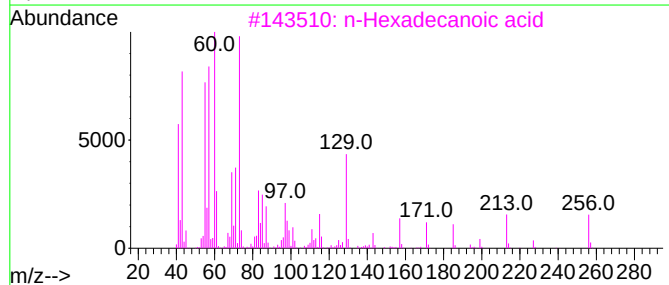
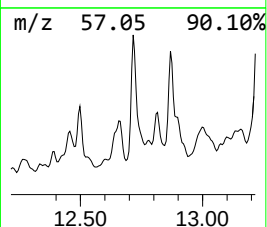
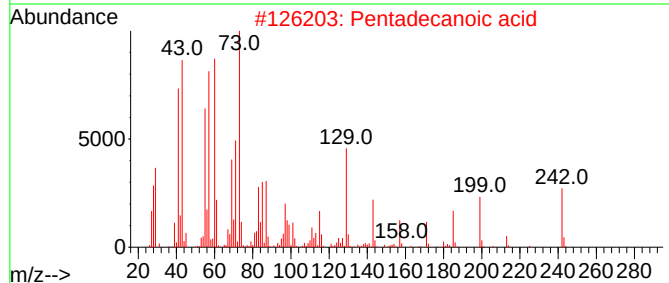
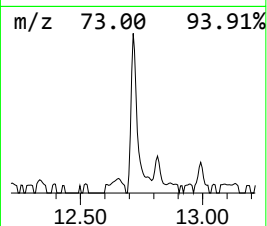
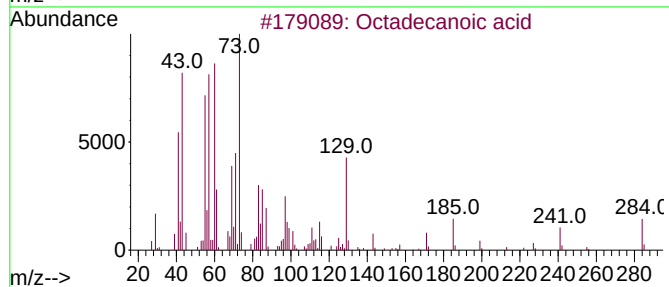
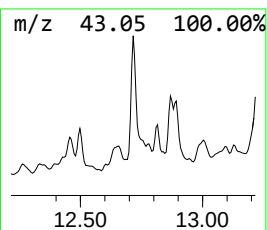
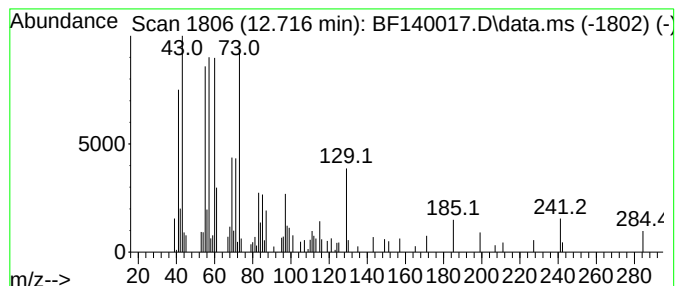
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.63 ng	74457	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140017.D
Acq On : 24 Oct 2024 22:58
Operator : RC/JU
Sample : P4487-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

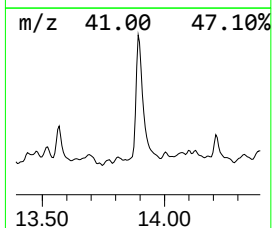
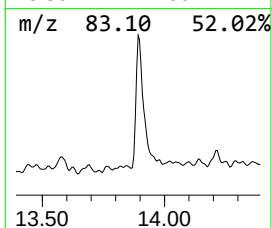
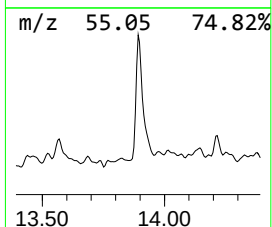
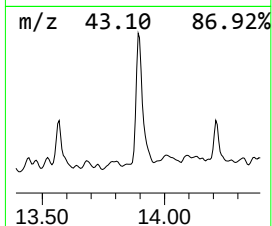
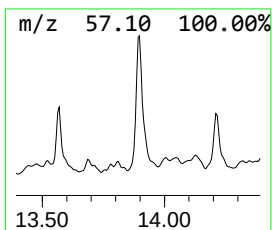
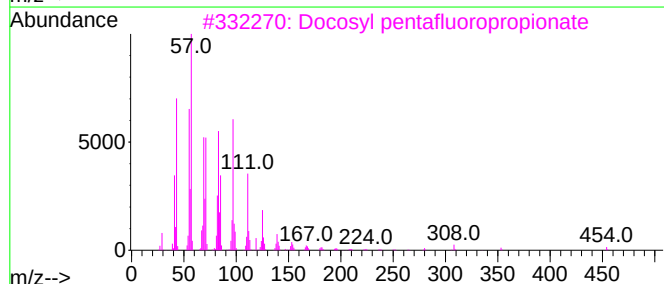
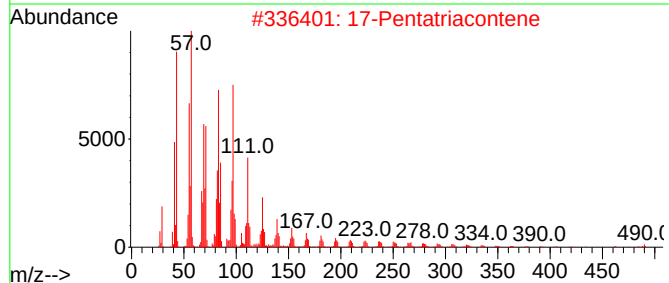
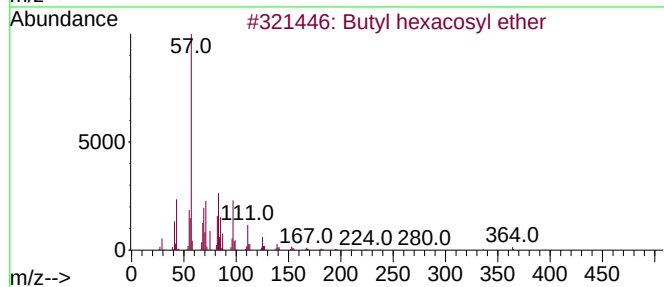
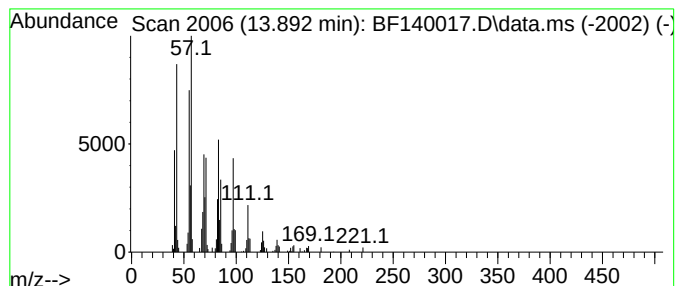
Instrument :
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ClientSampleId :
BP-B5

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 8 Butyl hexacosyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.892	7.47 ng	146296	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl hexacosyl ether	438	C30H62O	1000406-41-0	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140017.D
Acq On : 24 Oct 2024 22:58
Operator : RC/JU
Sample : P4487-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-B5

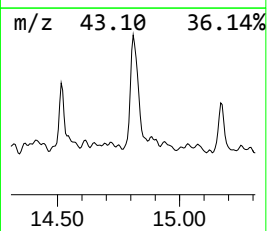
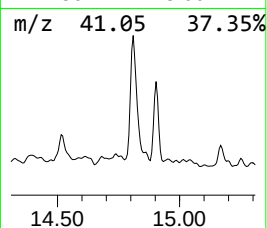
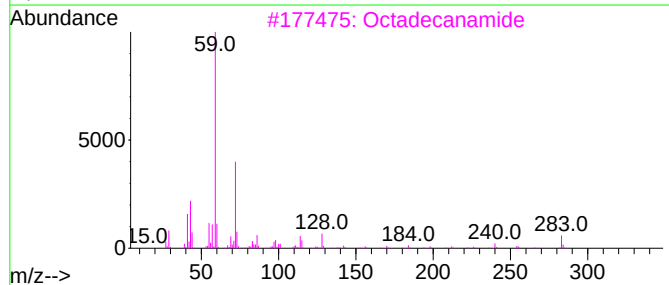
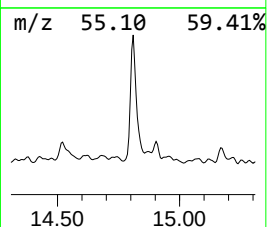
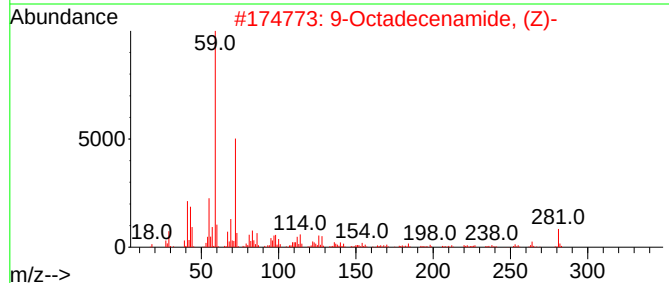
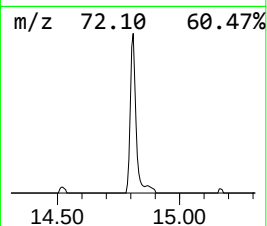
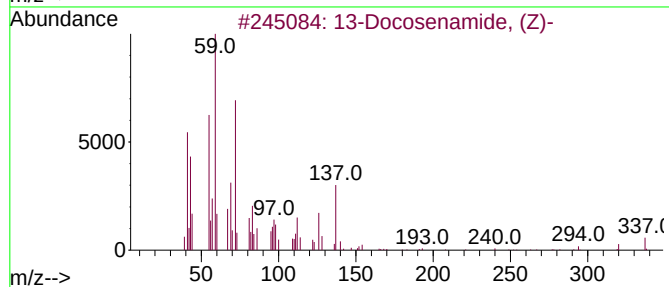
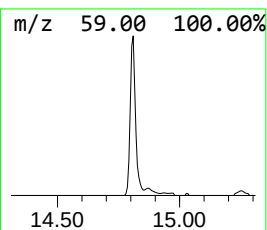
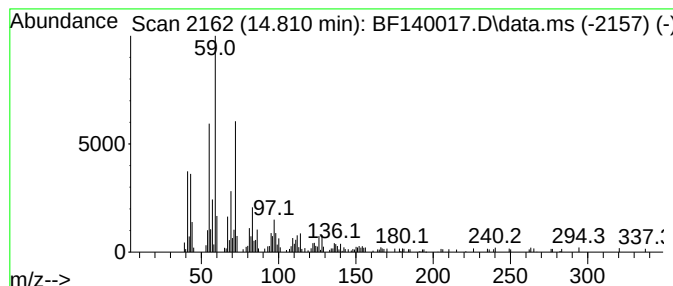
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	7.43 ng	188300	Perylene-d12	15.527

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	72
3			Octadecanamide	283	C18H37NO	000124-26-5	64
4			Decanamide-	171	C10H21NO	002319-29-1	50
5			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140017.D
Acq On : 24 Oct 2024 22:58
Operator : RC/JU
Sample : P4487-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-B5

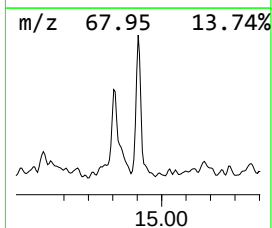
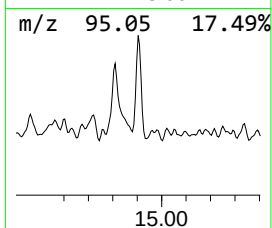
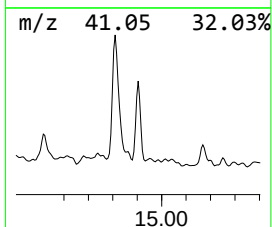
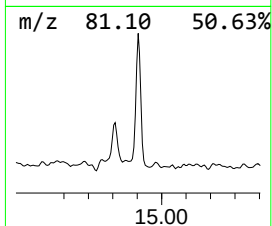
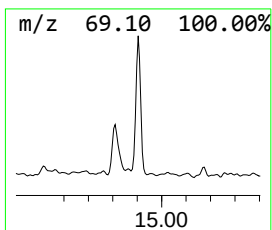
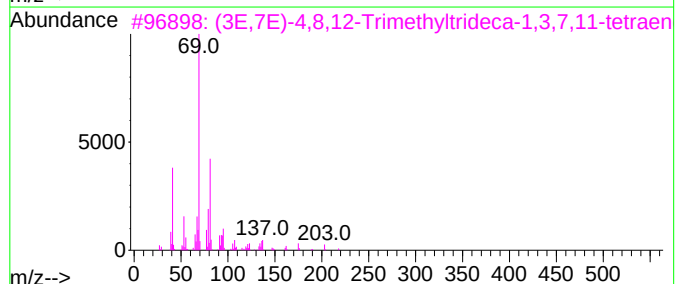
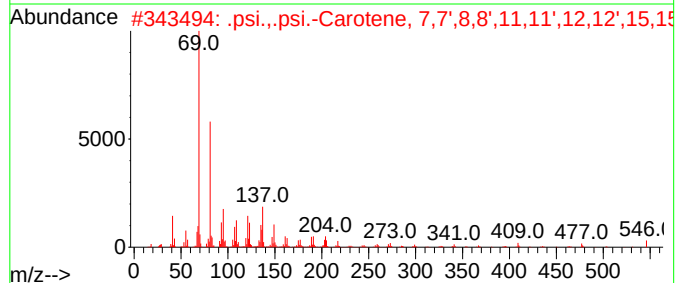
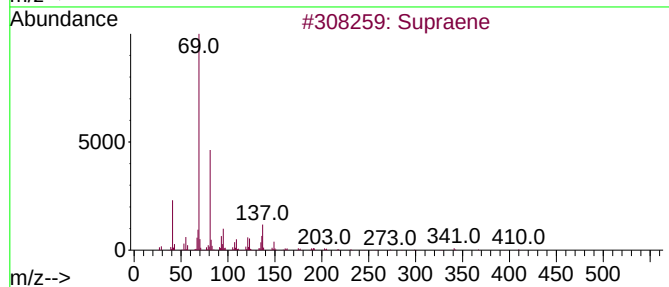
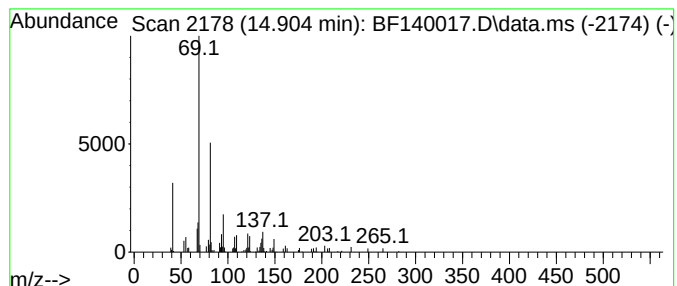
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	2.34 ng	59284	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
3			(3E,7E)-4,8,12-Trimethyltrideca-	218	C16H26	062235-06-7	72
4			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	64
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140017.D
Acq On : 24 Oct 2024 22:58
Operator : RC/JU
Sample : P4487-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Butenal, 3-me...	5.992	3.7	ng	89066	1	6.886	484092	20.0
Pentanedioic ac...	7.698	2.2	ng	69247	2	8.169	621923	20.0
Benzophenone	10.633	15.3	ng	502537	3	9.922	655489	20.0
Methanone, (1-h...	10.945	2.3	ng	63823	4	11.410	566983	20.0
n-Hexadecanoic ...	11.933	12.3	ng	348248	4	11.410	566983	20.0
Octadecanoic acid	12.716	2.6	ng	74457	4	11.410	566983	20.0
Butyl hexacosyl...	13.892	7.5	ng	146296	5	14.045	391858	20.0
13-Docosenamide...	14.810	7.4	ng	188300	6	15.527	506693	20.0
Supraene	14.904	2.3	ng	59284	6	15.527	506693	20.0