

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
 Data File : BF129990.D
 Acq On : 25 Aug 2022 01:38
 Operator : CG\JU
 Sample : N4264-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 U-3

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-BF081422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129990.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.410	528	531	550	rBV	750111	884201	24.91%	5.004%
2	6.434	702	705	719	rBV	431021	540331	15.22%	3.058%
3	6.763	758	761	770	rBV	731027	623048	17.55%	3.526%
4	7.334	854	858	869	rBV	1952629	1934566	54.50%	10.947%
5	7.816	937	940	948	rBV2	33188	43237	1.22%	0.245%
6	7.957	961	964	972	rBV	36447	50795	1.43%	0.287%
7	8.045	976	979	983	rBV	953430	797690	22.47%	4.514%
8	8.416	1038	1042	1050	rBV	87811	97173	2.74%	0.550%
9	9.122	1155	1162	1165	rBV	4295591	3549641	100.00%	20.087%
10	9.798	1273	1277	1281	rVB	1035197	830335	23.39%	4.699%
11	10.016	1311	1314	1323	rBV	49497	65263	1.84%	0.369%
12	10.181	1338	1342	1345	rBV	2351310	1884827	53.10%	10.666%
13	10.598	1409	1413	1420	rBV	1407412	1236041	34.82%	6.995%
14	11.286	1527	1530	1534	rBV	819569	714545	20.13%	4.043%
15	11.810	1615	1619	1623	rBV	62760	75799	2.14%	0.429%
16	12.869	1795	1799	1803	rBV	2740627	2477998	69.81%	14.023%
17	13.692	1935	1939	1941	rBV	88488	75126	2.12%	0.425%
18	13.722	1941	1944	1947	rVV	259836	222129	6.26%	1.257%
19	13.774	1947	1953	1964	rVB6	29632	79970	2.25%	0.453%
20	13.933	1977	1980	1985	rBV	577399	538251	15.16%	3.046%
21	14.022	1991	1995	2000	rBV	302233	303681	8.56%	1.718%
22	14.674	2102	2106	2109	rBV3	36429	42175	1.19%	0.239%
23	15.386	2223	2227	2236	rVB	482696	604636	17.03%	3.422%

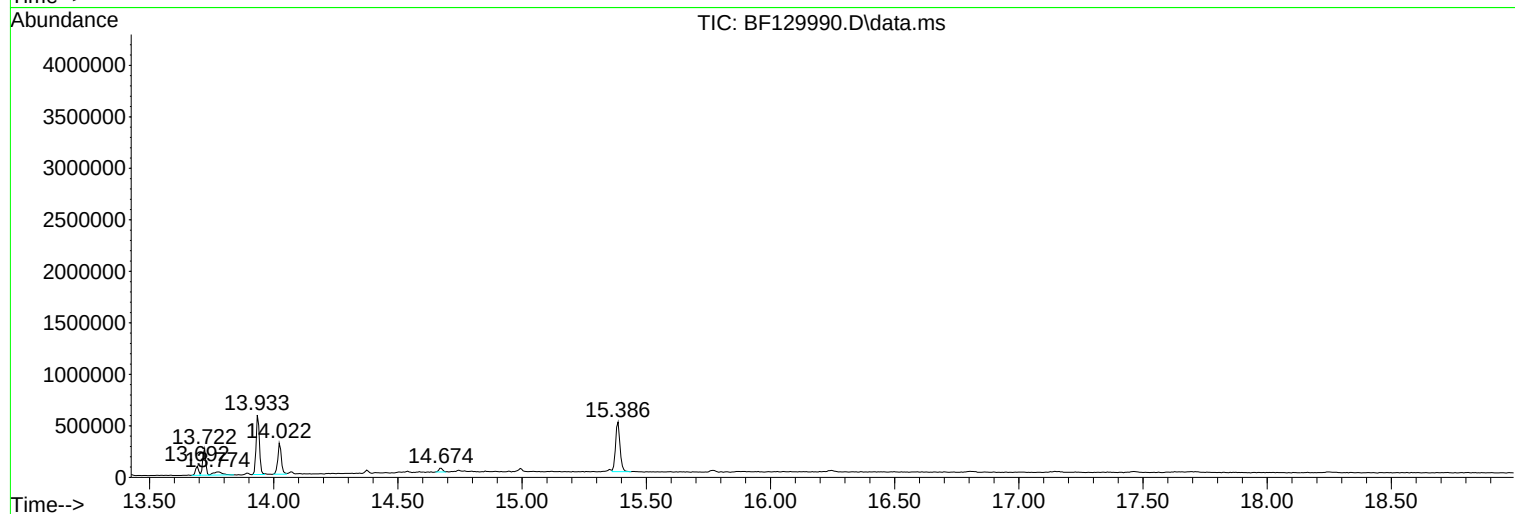
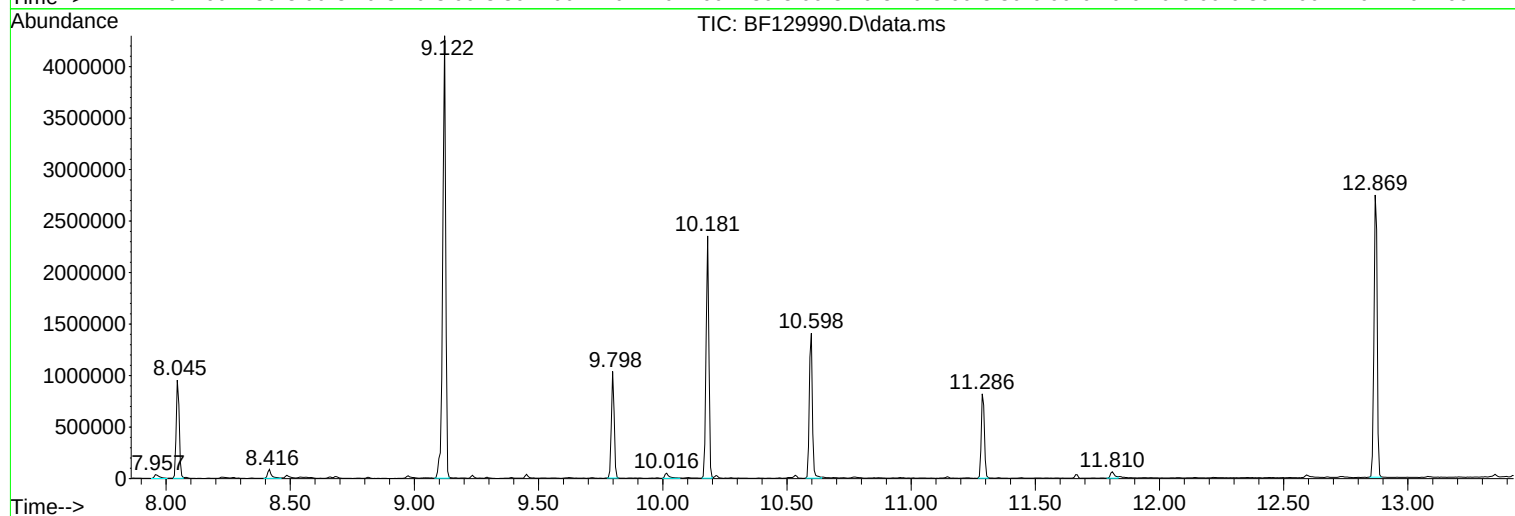
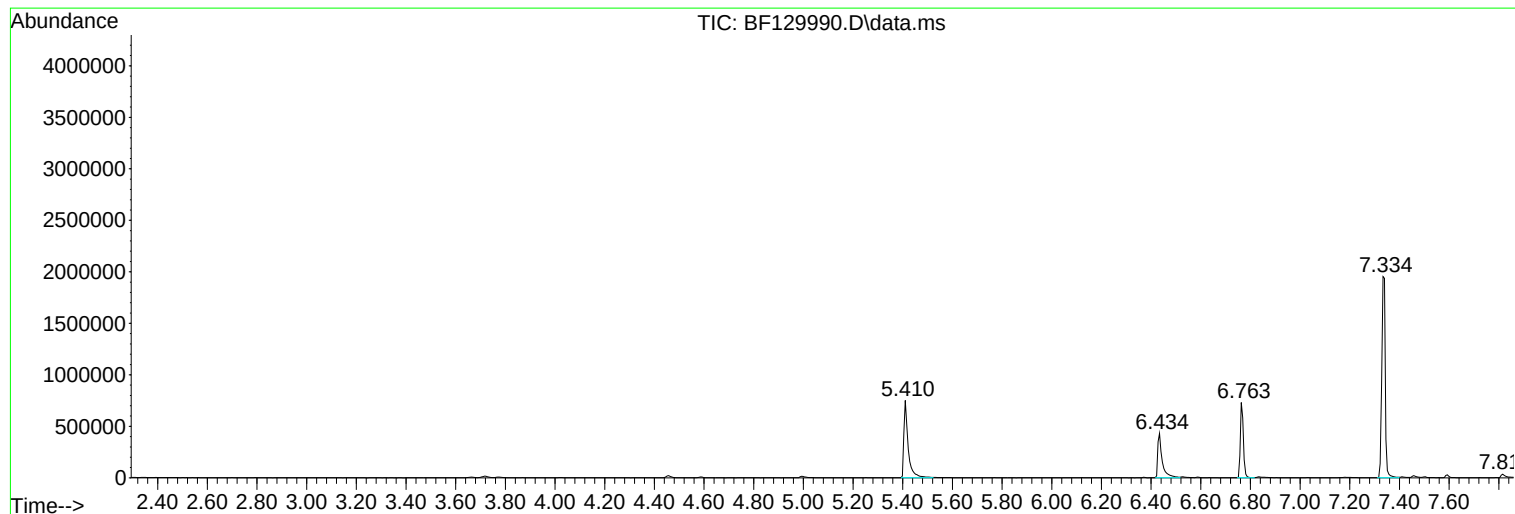
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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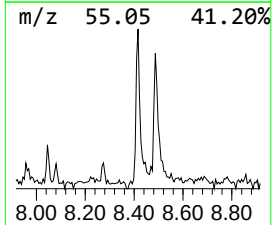
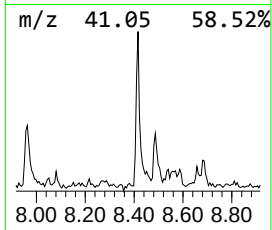
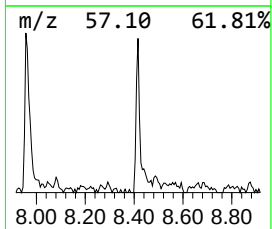
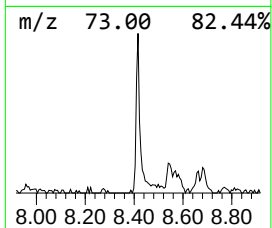
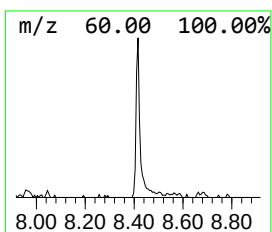
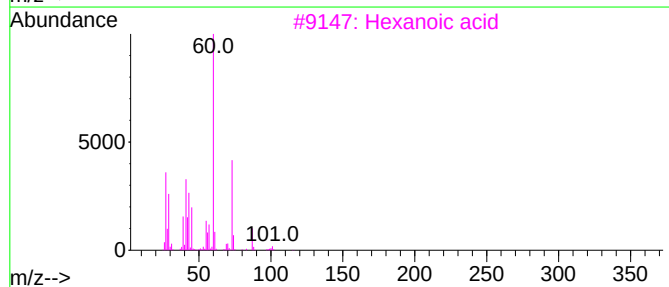
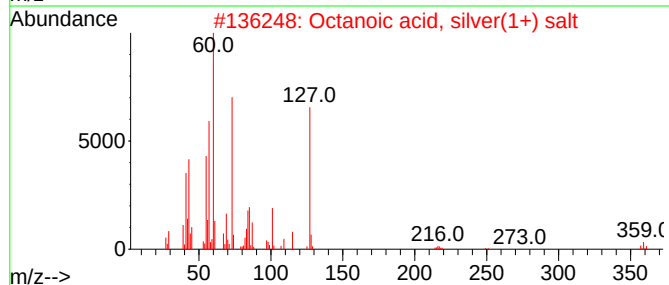
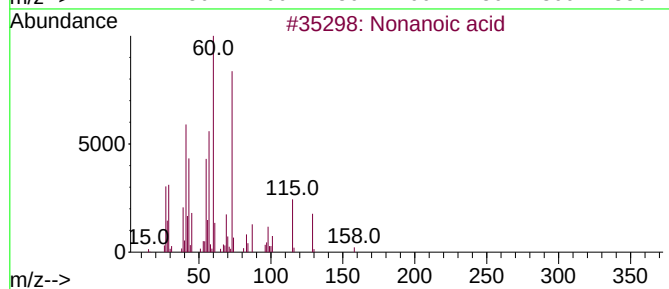
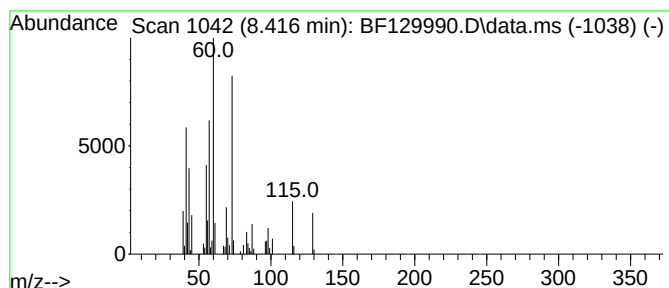
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Nonanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.416	2.44 ng	97173	Naphthalene-d8	8.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	91
2			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	53
3			Hexanoic acid	116	C6H12O2	000142-62-1	53
4			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	47
5			5-Methylhexanoic acid	130	C7H14O2	000628-46-6	47



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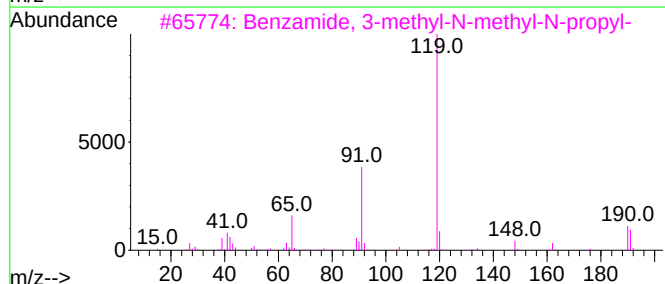
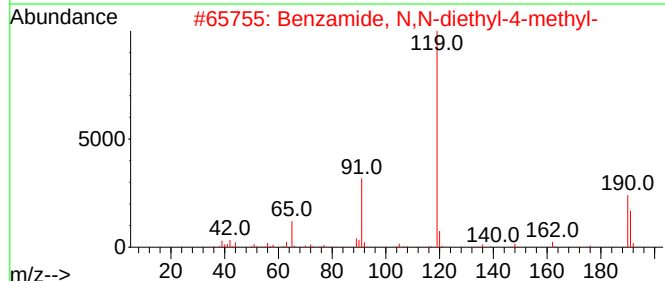
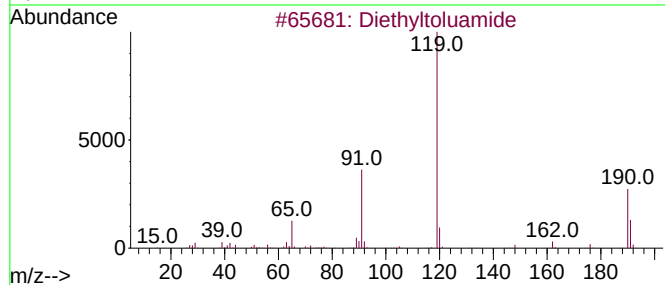
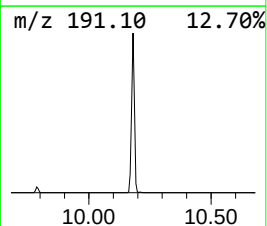
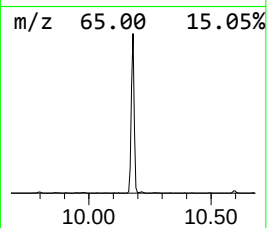
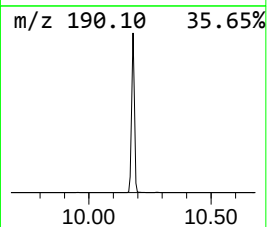
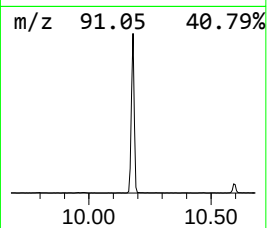
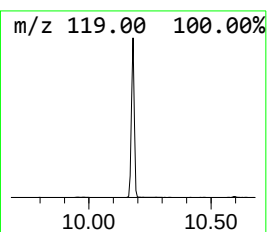
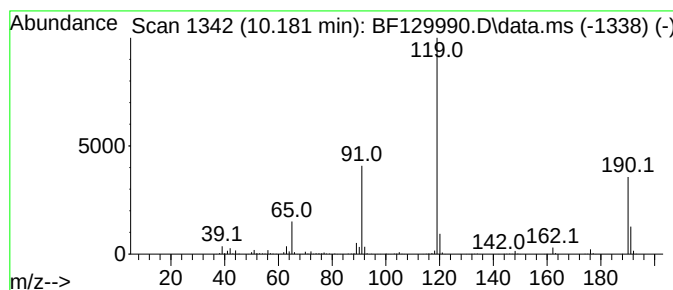
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Peak Number 2 Diethyltoluamide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.181	45.40 ng	1884830	Acenaphthene-d10	9.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyltoluamide	191	C12H17NO	000134-62-3	96
2			Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	90
3			Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	90
4			Benzamide, 2-methyl-N-methyl-N-p...	191	C12H17NO	1000421-44-4	87
5			Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	87



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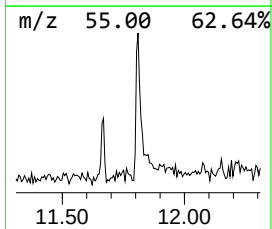
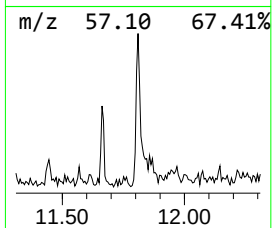
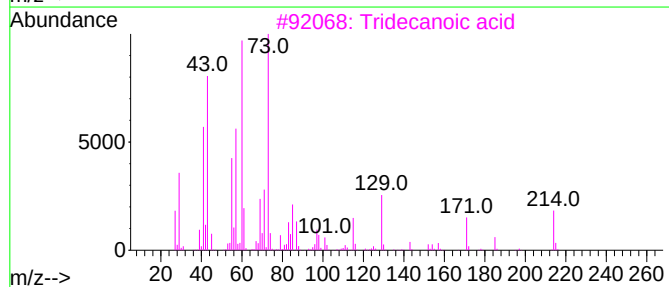
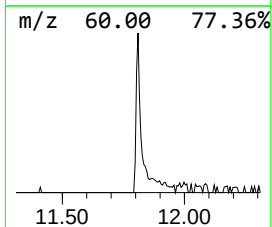
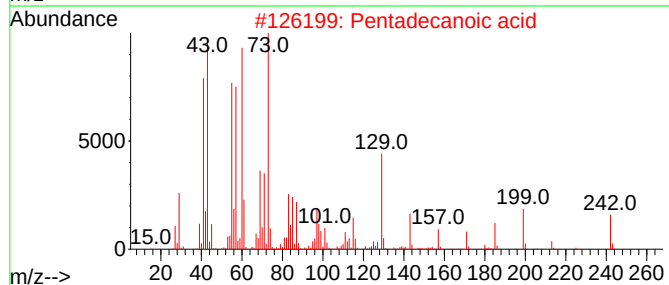
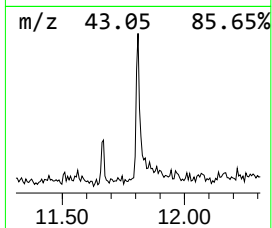
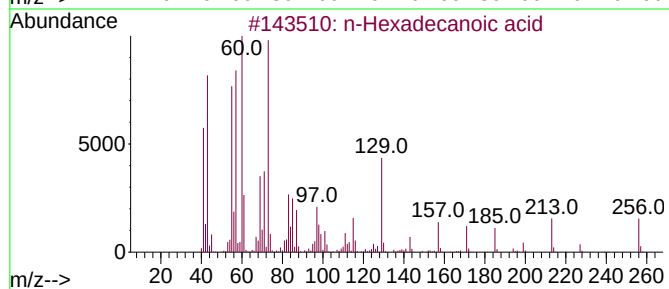
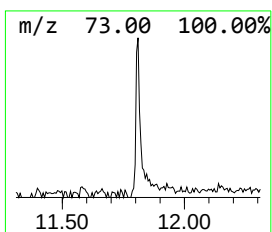
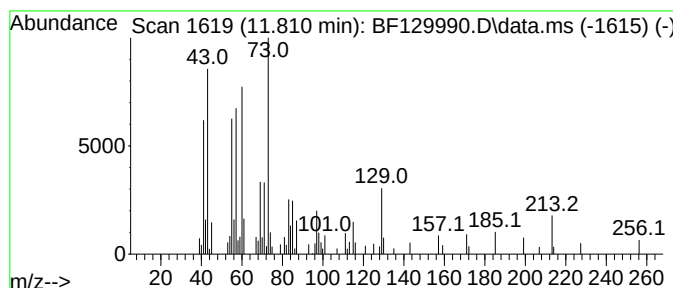
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.810	2.12 ng	75799	Phenanthrene-d10	11.286	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60



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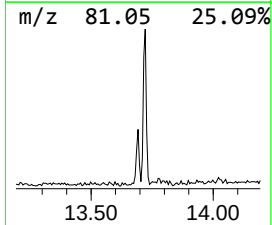
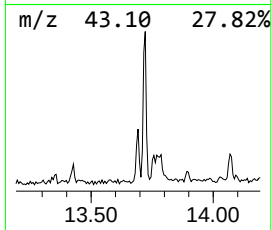
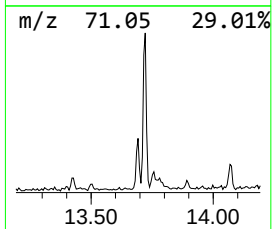
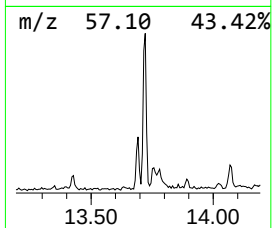
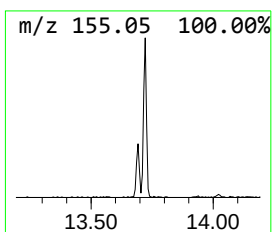
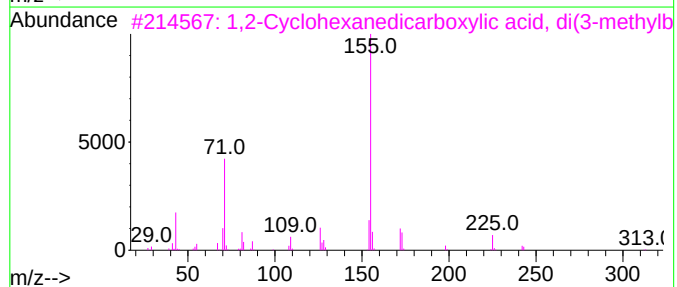
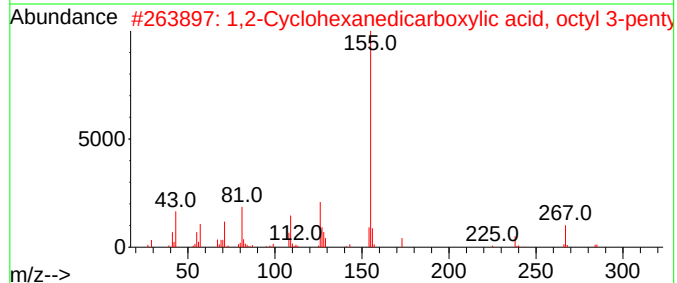
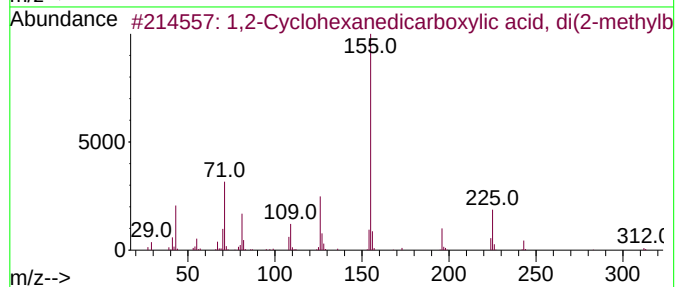
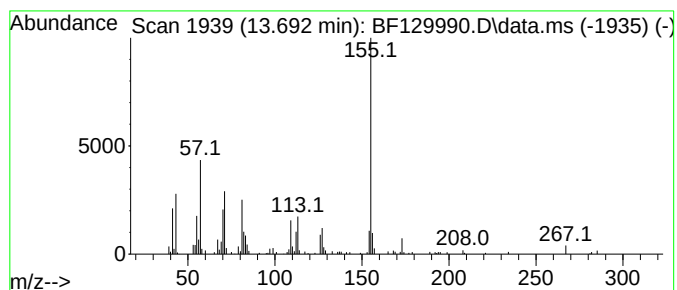
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Peak Number 4 1,2-Cyclohexanedicarboxylic... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.692	2.79 ng	75126	Chrysene-d12	13.933	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclohexanedicarboxylic acid...	312	C18H32O4	1000339-55-6	59
2	1,2-Cyclohexanedicarboxylic acid...	354	C21H38O4	1000339-50-6	53
3	1,2-Cyclohexanedicarboxylic acid...	312	C18H32O4	1000339-57-1	53
4	1,2-Cyclohexanedicarboxylic acid...	366	C22H38O4	1000339-76-4	50
5	1,2-Cyclohexanedicarboxylic acid...	310	C18H30O4	1000339-75-9	50



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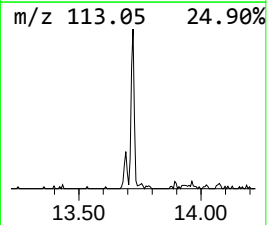
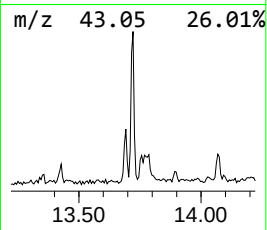
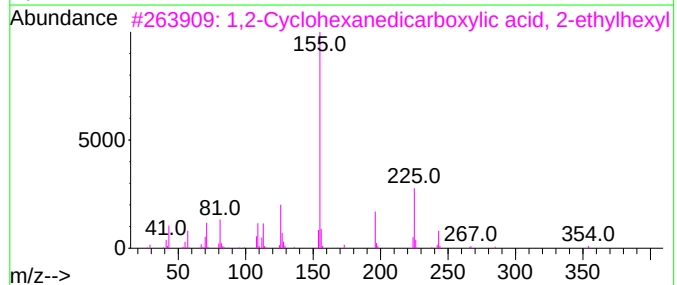
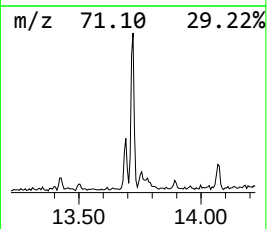
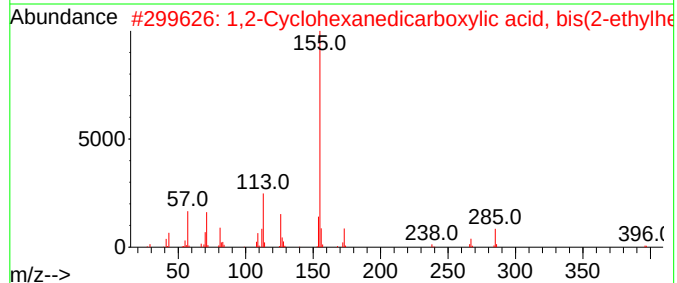
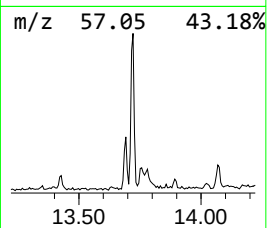
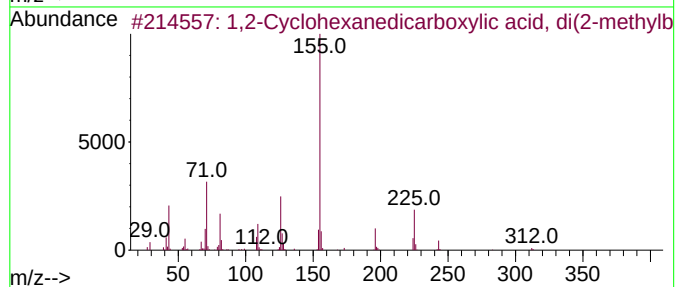
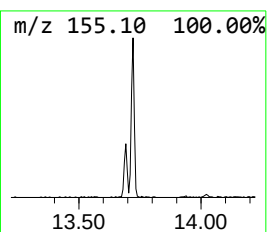
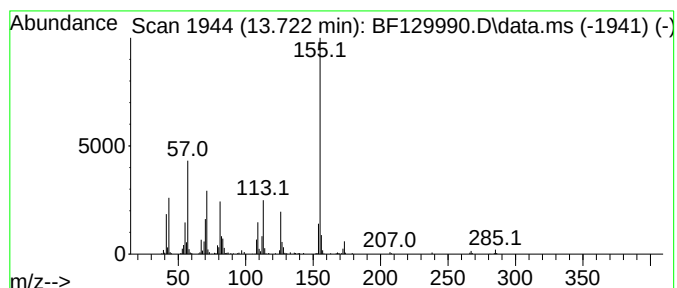
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Peak Number 5 unknown13.722 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.722	8.25 ng	222129	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Cyclohexanedicarboxylic acid...	312	C18H32O4	1000339-55-6	80
2			1,2-Cyclohexanedicarboxylic acid...	396	C24H44O4	000084-71-9	72
3			1,2-Cyclohexanedicarboxylic acid...	354	C21H38O4	1000339-45-4	64
4			1,2-Cyclohexanedicarboxylic acid...	354	C21H38O4	1000339-54-8	59
5			1,2-Cyclohexanedicarboxylic acid...	354	C21H38O4	1000339-50-6	59



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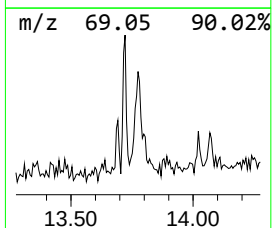
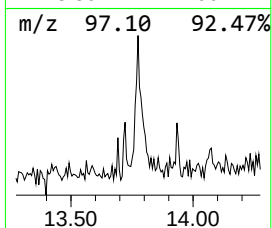
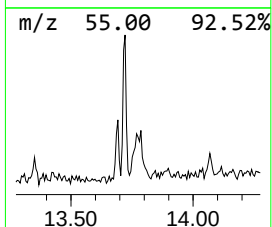
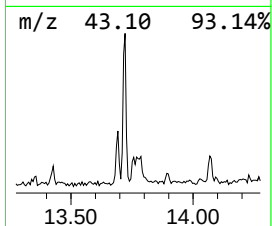
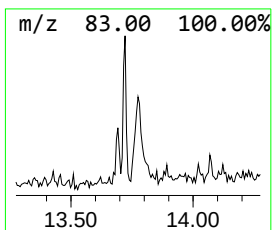
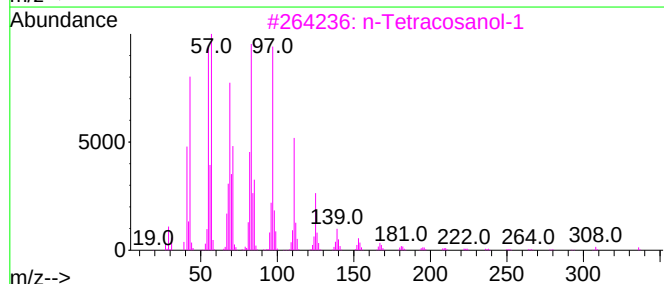
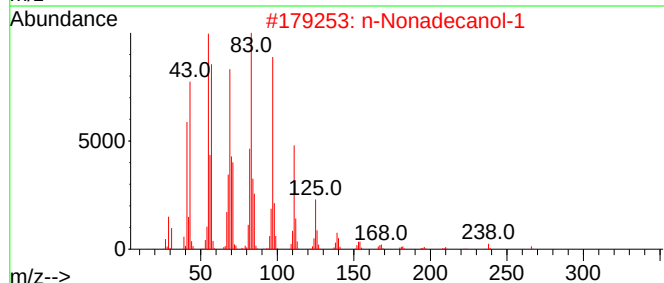
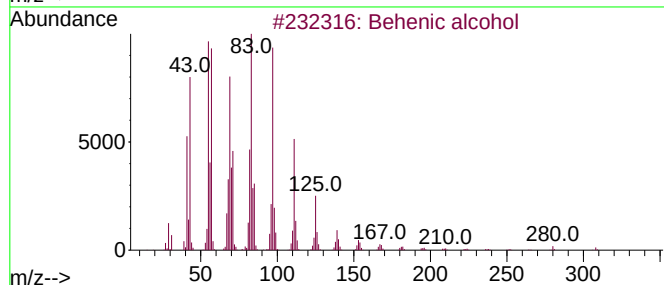
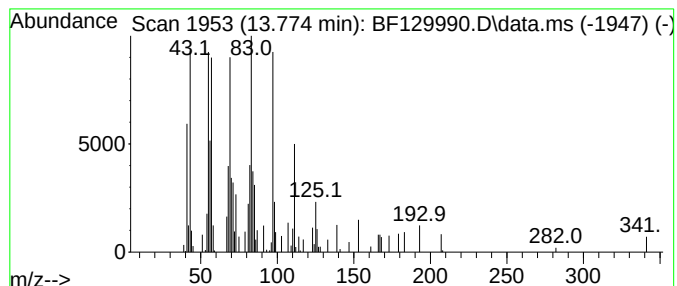
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.775	2.97 ng	79970	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	91
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
Data File : BF129990.D
Acq On : 25 Aug 2022 01:38
Operator : CG\JU
Sample : N4264-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

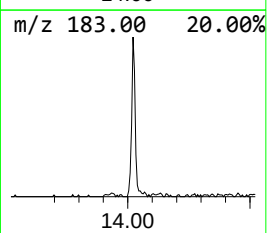
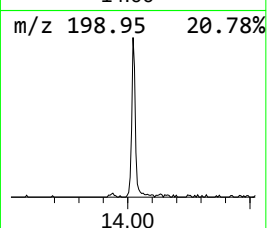
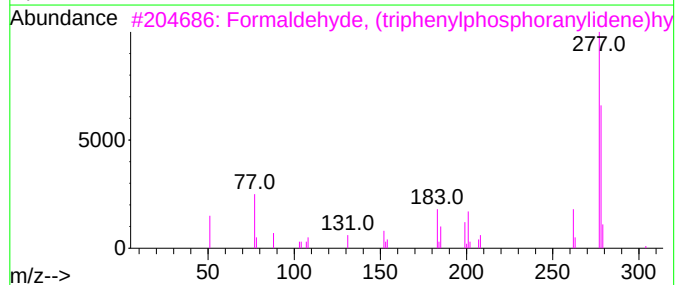
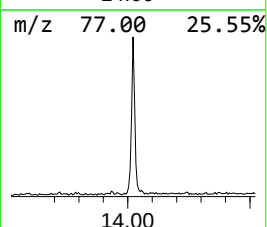
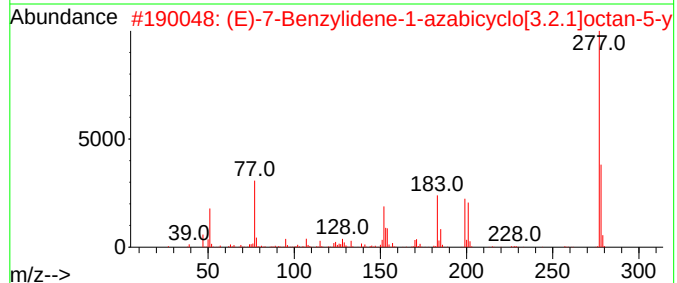
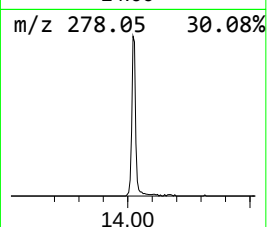
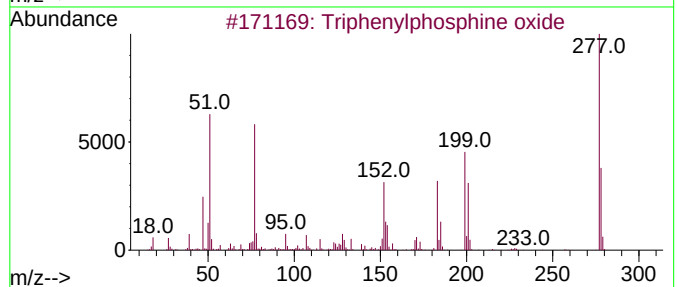
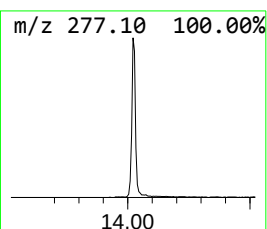
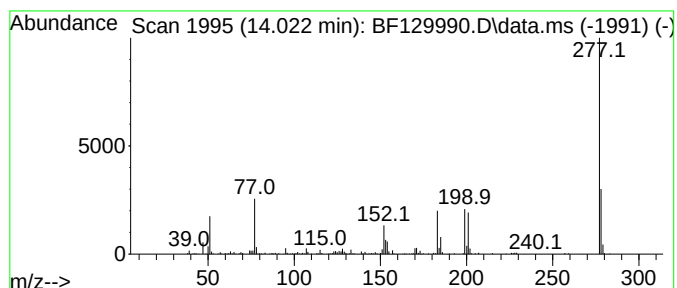
Instrument :
BNA_F
ClientSampleId :
U-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.022	11.28 ng	303681	Chrysene-d12	13.933	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	76
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	38
5	1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19N03Si	072101-35-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
Data File : BF129990.D
Acq On : 25 Aug 2022 01:38
Operator : CG\JU
Sample : N4264-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
U-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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
Nonanoic acid	8.416	2.4	ng	97173	2	8.045	797690	20.0
Diethyltoluamide	10.181	45.4	ng	1884830	3	9.798	830335	20.0
n-Hexadecanoic ...	11.810	2.1	ng	75799	4	11.286	714545	20.0
1,2-Cyclohexane...	13.692	2.8	ng	75126	5	13.933	538251	20.0
unknown13.722	13.722	8.3	ng	222129	5	13.933	538251	20.0
Behenic alcohol	13.775	3.0	ng	79970	5	13.933	538251	20.0
Triphenylphosph...	14.022	11.3	ng	303681	5	13.933	538251	20.0