

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
 Data File : BF128613.D
 Acq On : 01 Jun 2022 00:36
 Operator : CG\JU
 Sample : N2952-30
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P043-SS001-0612-02

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128613.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.516	545	549	561	rBV	1846379	2307612	87.48%	13.813%
2	6.534	718	722	743	rVB	1732987	2255947	85.52%	13.504%
3	6.845	771	775	778	rBV	676275	567423	21.51%	3.396%
4	7.410	865	871	874	rBV	1679162	1532548	58.10%	9.174%
5	7.592	899	902	906	rVB	46649	39373	1.49%	0.236%
6	8.128	989	993	996	rBV	827213	660628	25.04%	3.954%
7	9.204	1171	1176	1179	rBV	3248092	2637811	100.00%	15.789%
8	9.463	1218	1220	1223	rVB	40948	36558	1.39%	0.219%
9	9.880	1287	1291	1295	rBV	753177	662525	25.12%	3.966%
10	10.680	1423	1427	1430	rBV	1604275	1375506	52.15%	8.234%
11	11.369	1541	1544	1548	rBV	679672	606677	23.00%	3.631%
12	11.904	1632	1635	1643	rBV2	128413	163992	6.22%	0.982%
13	12.574	1745	1749	1754	rBV3	103094	145181	5.50%	0.869%
14	12.692	1766	1769	1774	rBV4	36268	43911	1.66%	0.263%
15	12.963	1810	1815	1818	rBV	2495866	2226307	84.40%	13.326%
16	13.351	1876	1881	1888	rVB3	74010	110093	4.17%	0.659%
17	13.592	1919	1922	1926	rBV	33472	40988	1.55%	0.245%
18	13.904	1972	1975	1981	rBV6	34518	60406	2.29%	0.362%
19	14.015	1988	1994	1997	rBV	533385	548567	20.80%	3.284%
20	14.063	1997	2002	2006	rVV4	60158	92291	3.50%	0.552%
21	14.110	2007	2010	2015	rVB	151211	162559	6.16%	0.973%
22	14.780	2121	2124	2130	rBV4	70012	87042	3.30%	0.521%
23	15.486	2240	2244	2248	rBV	289658	342264	12.98%	2.049%

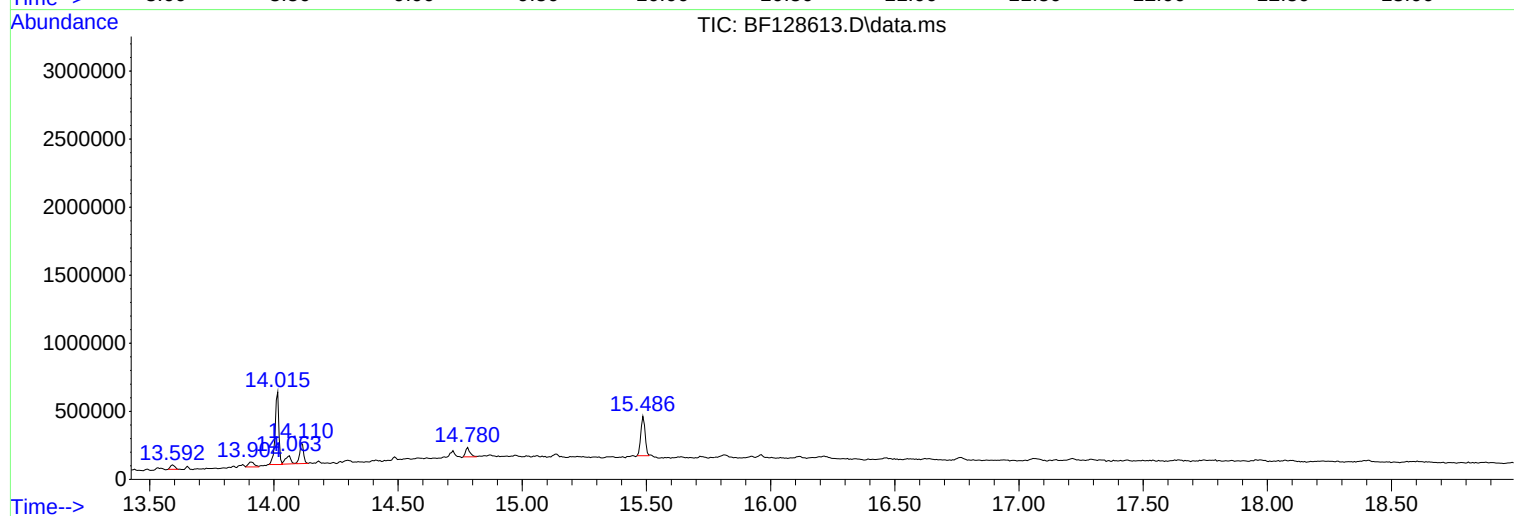
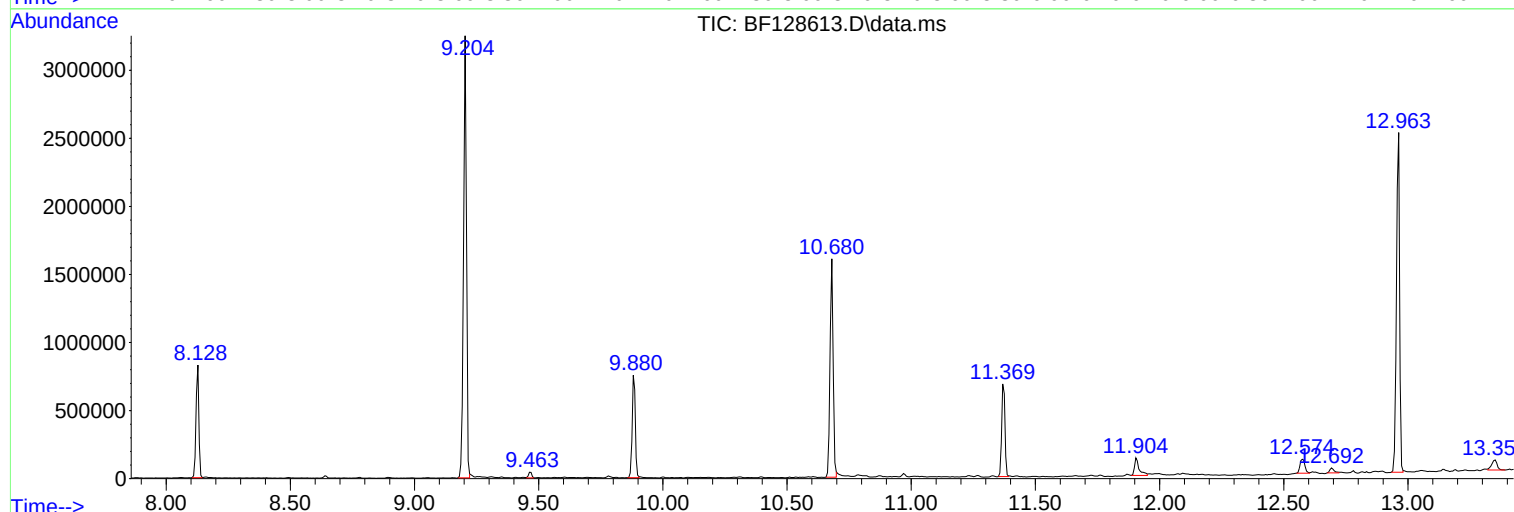
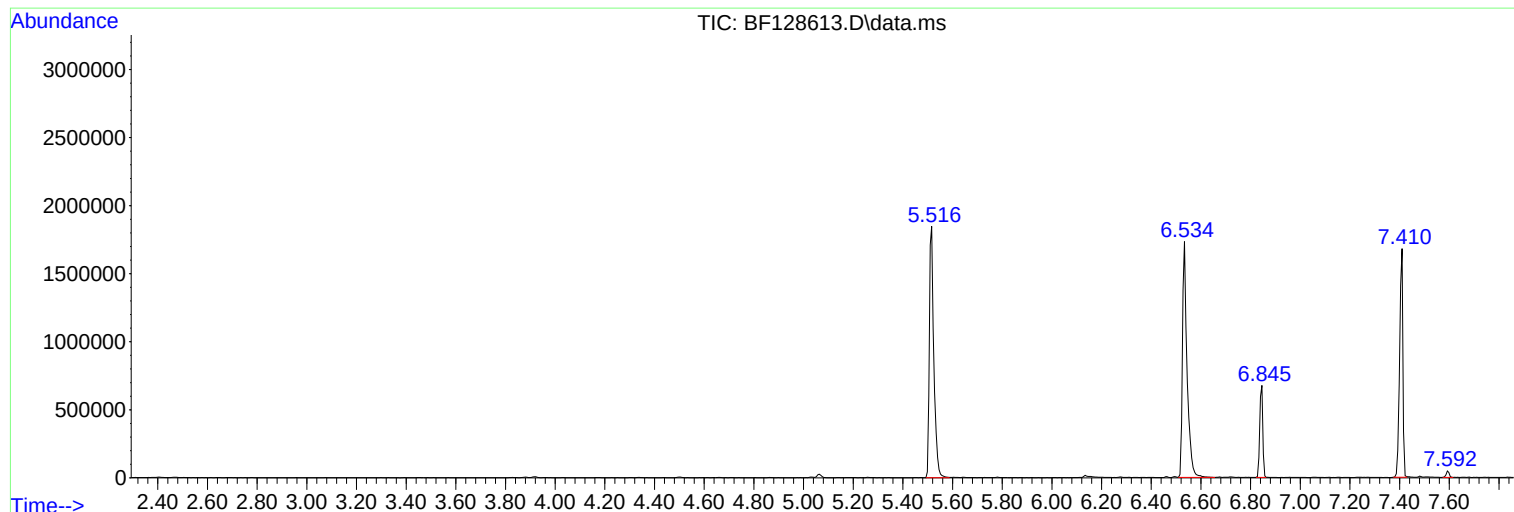
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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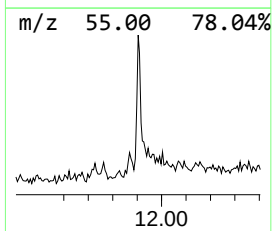
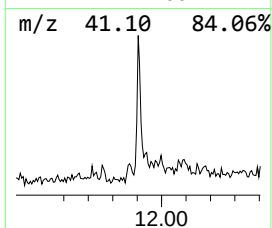
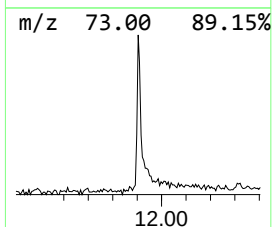
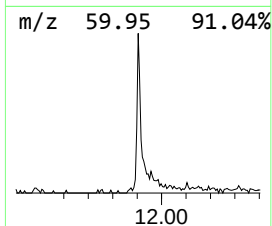
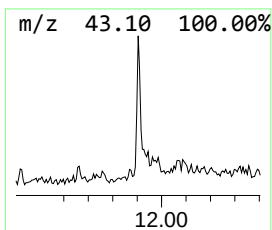
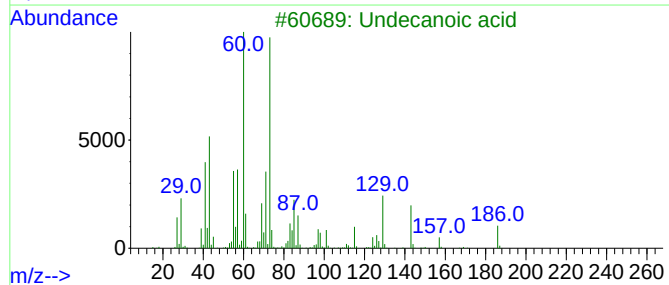
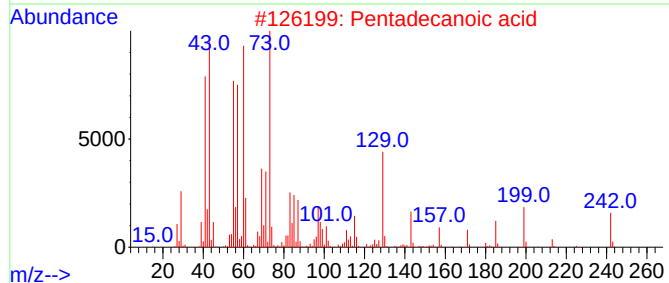
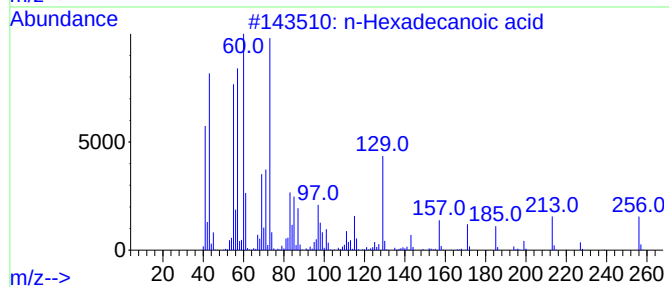
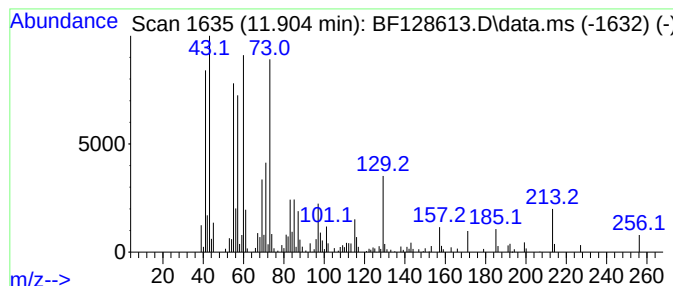
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	5.41 ng	163992	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3			Undecanoic acid	186	C11H22O2	000112-37-8	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	53



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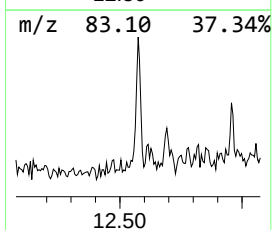
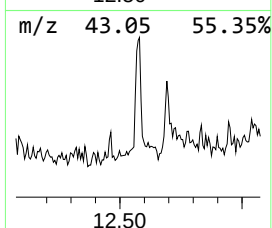
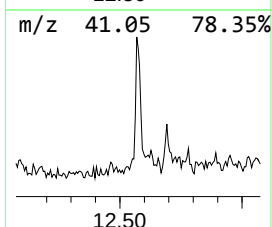
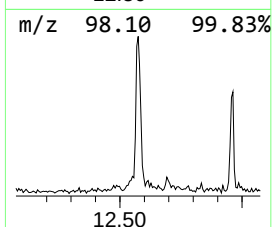
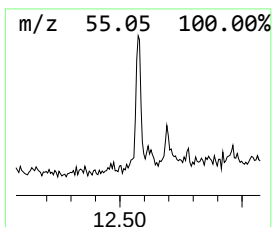
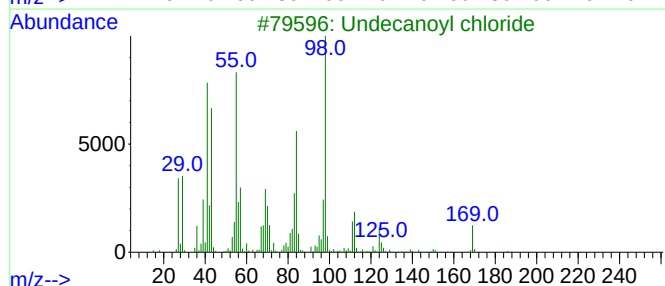
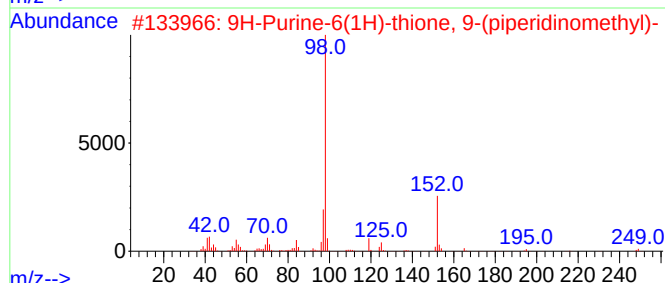
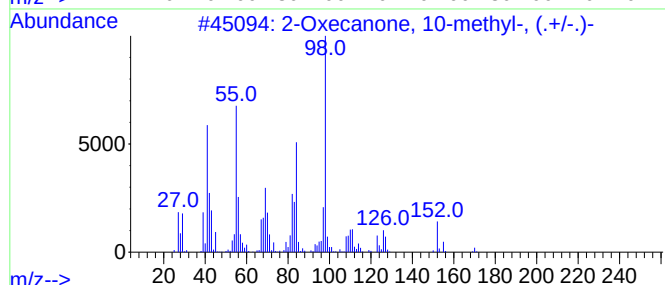
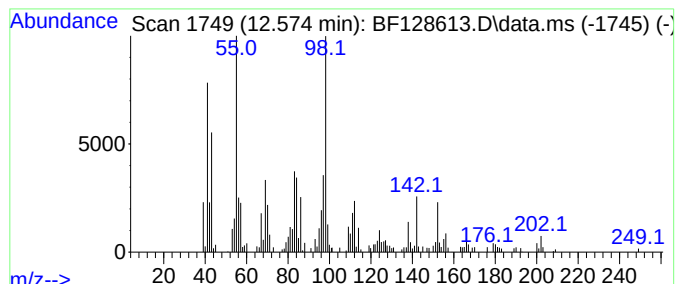
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Peak Number 2 unknown12.574 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.574	4.79 ng	145181	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Oxecanone, 10-methyl-, (.+/-.)-	170	C10H18O2	065371-24-6	45
2			9H-Purine-6(1H)-thione, 9-(piper...	249	C11H15N5S	014133-14-3	43
3			Undecanoyl chloride	204	C11H21ClO	017746-05-3	38
4			2-(1-Methyl-3-butenyl)cyclohexanone	166	C11H18O	1000424-67-7	38
5			n-Heptylamine, N-acetyl-1-cyano-	182	C10H18N2O	1000227-03-9	35



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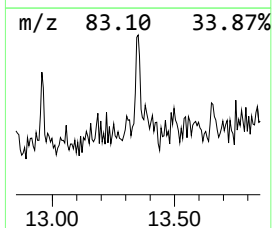
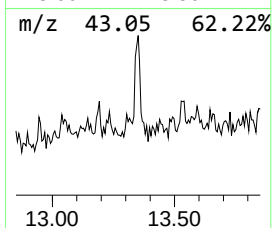
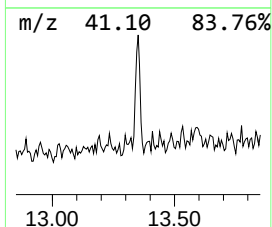
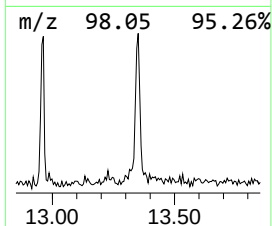
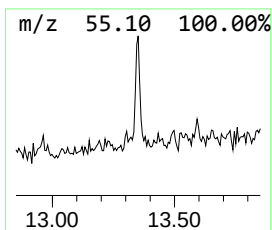
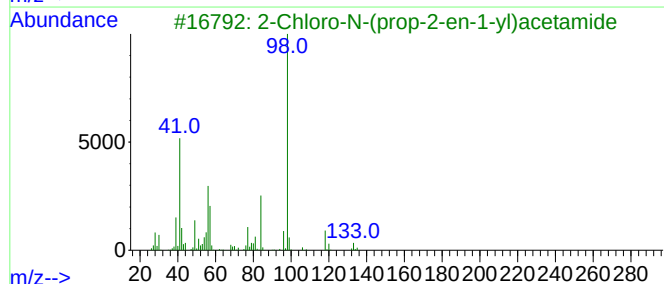
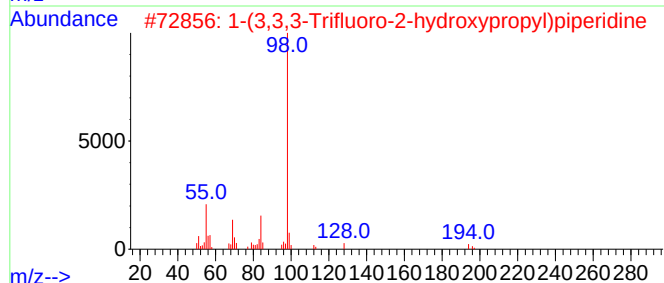
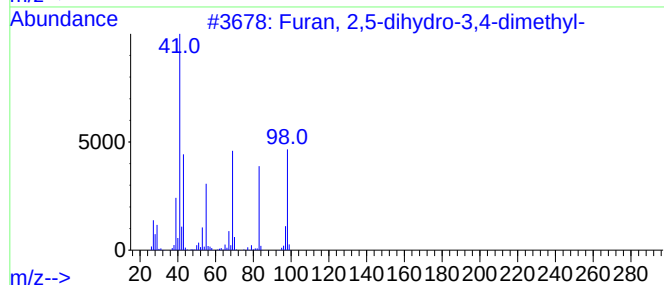
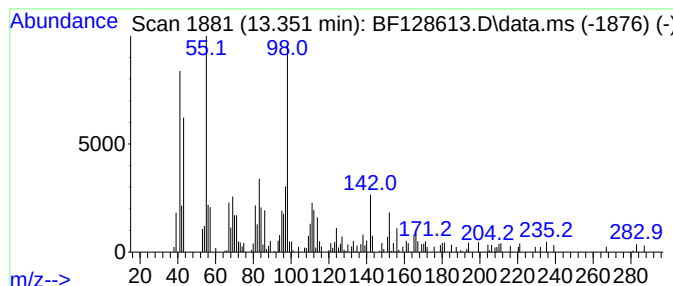
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Peak Number 3 unknown13.351 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.351	4.01 ng	110093	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,5-dihydro-3,4-dimethyl-	98	C6H10O	053720-72-2	30
2			1-(3,3,3-Trifluoro-2-hydroxypropyl)piperidine	197	C8H14F3NO	1000283-75-5	27
3			2-Chloro-N-(prop-2-en-1-yl)acetamide	133	C5H8ClNO	013269-97-1	27
4			2(3H)-Furanone, 5-methyl-	98	C5H6O2	000591-12-8	25
5			2-(1-Methyl-3-butenyl)cyclohexanone	166	C11H18O	1000424-67-7	25



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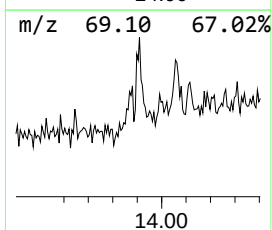
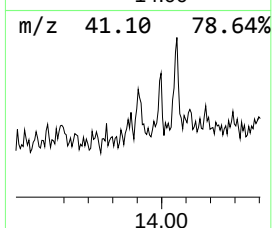
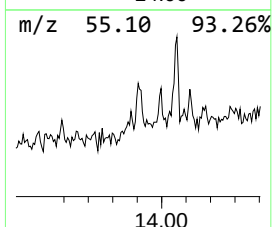
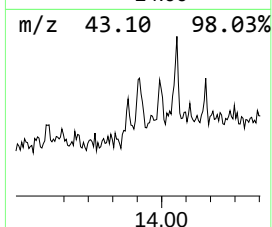
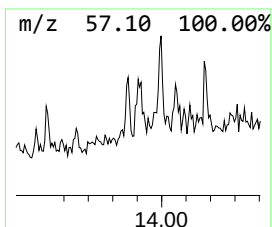
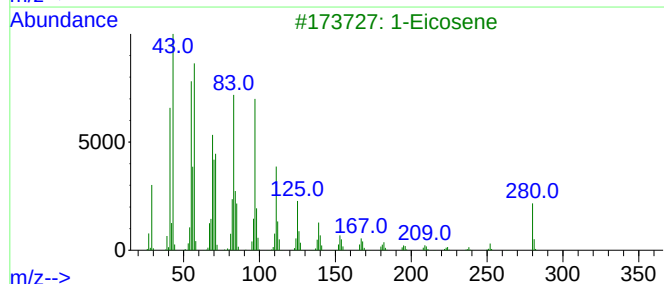
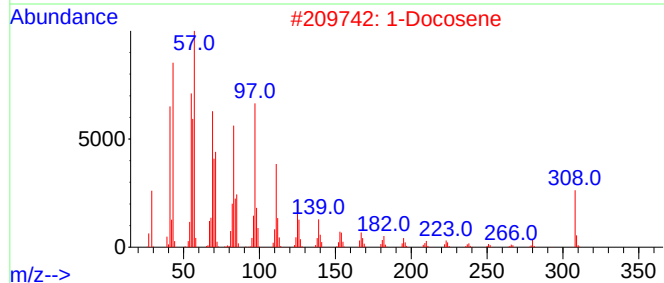
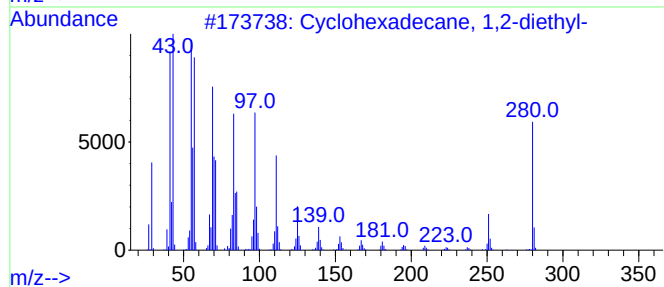
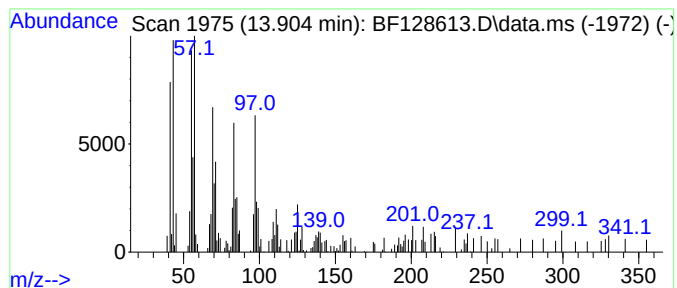
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Peak Number 4 Cyclohexadecane, 1,2-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.20 ng	60406	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	90
2			1-Docosene	308	C22H44	001599-67-3	89
3			1-Eicosene	280	C20H40	003452-07-1	83
4			Cycloeicosane	280	C20H40	000296-56-0	83
5			1-Tetracosene	336	C24H48	010192-32-2	76



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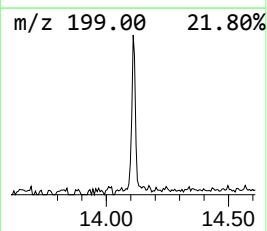
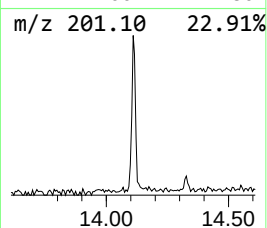
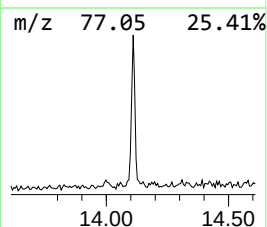
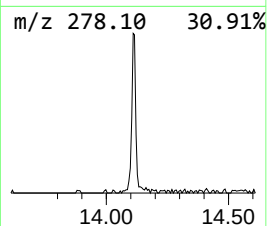
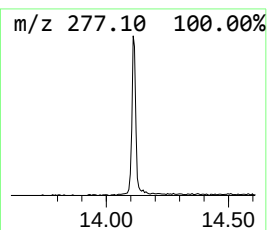
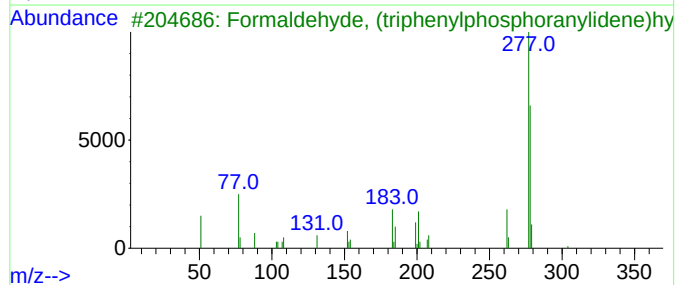
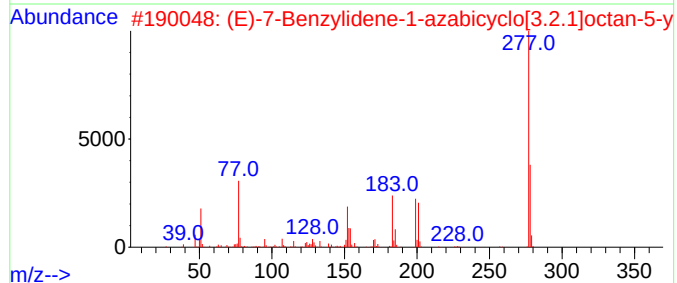
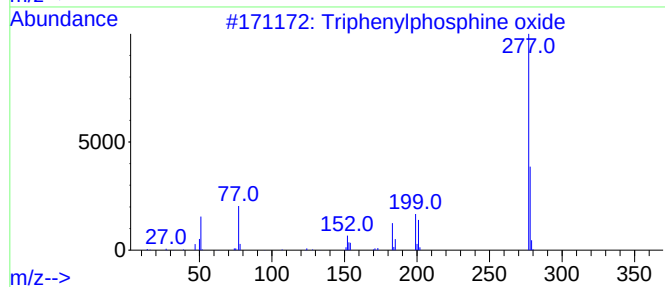
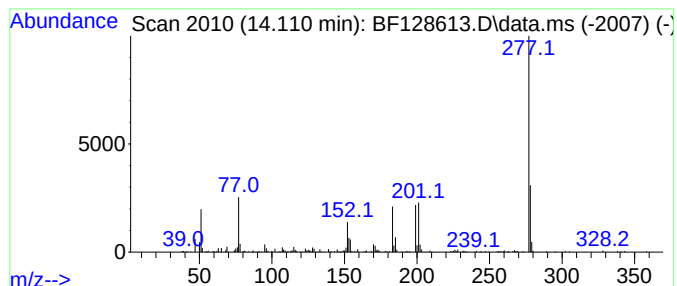
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	5.93 ng	162559	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	53
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	43
5			Furo[3,2-c]quinoline, 8-bromo-2,...	277	C13H12BrNO	1000310-92-7	37



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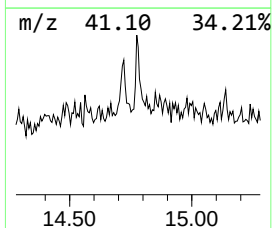
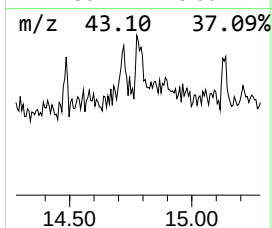
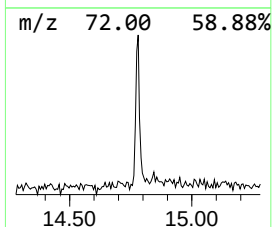
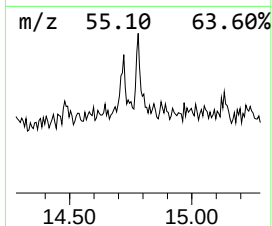
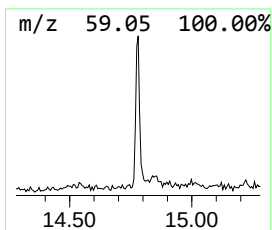
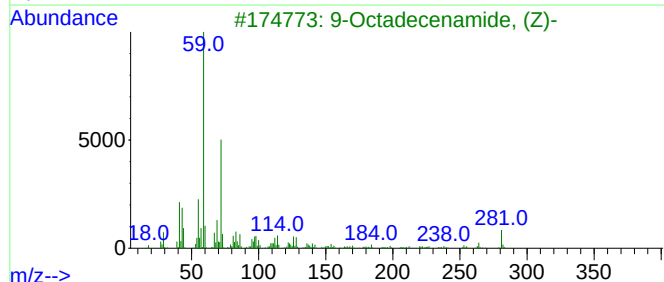
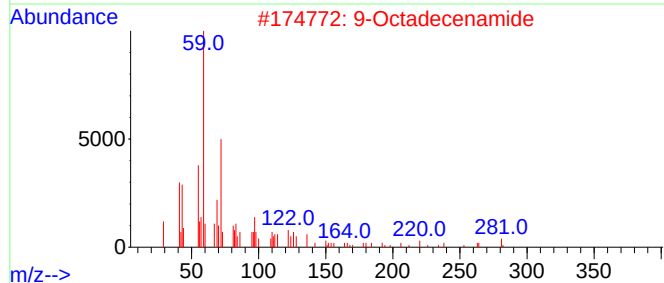
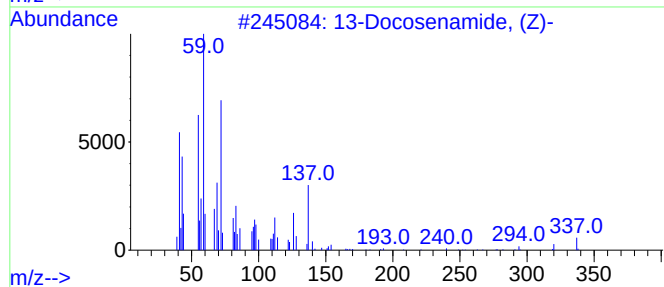
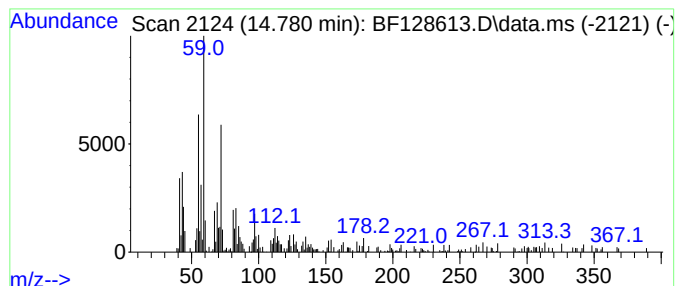
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	5.09 ng	87042	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2			9-Octadecenamide	281	C18H35NO	003322-62-1	80
3			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
4			Palmitoleamide	253	C16H31NO	106010-22-4	64
5			Hexadecanamide	255	C16H33NO	000629-54-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128613.D
Acq On : 01 Jun 2022 00:36
Operator : CG\JU
Sample : N2952-30
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P043-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
n-Hexadecanoic ...	11.904	5.4	ng	163992	4	11.369	606677	20.0
unknown12.574	12.574	4.8	ng	145181	4	11.369	606677	20.0
unknown13.351	13.351	4.0	ng	110093	5	14.015	548567	20.0
Cyclohexadecane...	13.904	2.2	ng	60406	5	14.015	548567	20.0
Triphenylphosph...	14.110	5.9	ng	162559	5	14.015	548567	20.0
13-Docosenamide...	14.780	5.1	ng	87042	6	15.486	342264	20.0