

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
 Data File : BF127921.D
 Acq On : 26 Apr 2022 19:15
 Operator : CG\JU
 Sample : N2551-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220375-096-21-01-ELUTRIATE

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-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127921.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.557	552	556	569	rBV	1169380	1173458	33.52%	4.927%
2	6.557	722	726	735	rBV	1012017	923253	26.38%	3.877%
3	6.940	787	791	795	rBV	1065130	882221	25.20%	3.704%
4	7.504	881	887	890	rBV	1903209	1800999	51.45%	7.562%
5	7.669	912	915	920	rVB2	40999	38913	1.11%	0.163%
6	8.222	1005	1009	1013	rBV	1255905	1155514	33.01%	4.852%
7	9.298	1187	1192	1195	rBV	3497783	3129134	89.40%	13.139%
8	9.369	1201	1204	1207	rVB	52253	44860	1.28%	0.188%
9	9.557	1233	1236	1242	rBV	59988	61305	1.75%	0.257%
10	9.869	1280	1289	1292	rBV7	17344	37582	1.07%	0.158%
11	9.986	1303	1309	1312	rBV	1436587	1380634	39.44%	5.797%
12	10.075	1319	1324	1327	rBV	41014	36435	1.04%	0.153%
13	10.775	1438	1443	1452	rBV	2049349	1906454	54.46%	8.005%
14	11.475	1558	1562	1566	rBV	1644585	1361917	38.91%	5.719%
15	11.639	1585	1590	1593	rBV	3711512	3500331	100.00%	14.698%
16	11.769	1607	1612	1620	rBV8	17764	41913	1.20%	0.176%
17	11.857	1624	1627	1630	rVB	208156	180351	5.15%	0.757%
18	11.986	1646	1649	1654	rBV	227923	235117	6.72%	0.987%
19	12.645	1759	1761	1765	rVB	87793	75206	2.15%	0.316%
20	13.063	1828	1832	1835	rBV	2078018	1947076	55.63%	8.176%
21	13.745	1946	1948	1953	rVB3	42081	42807	1.22%	0.180%
22	14.016	1989	1994	2004	rBV4	294544	832237	23.78%	3.495%
23	14.121	2008	2012	2016	rVV	841348	744467	21.27%	3.126%
24	15.639	2265	2270	2275	rBV	595840	798918	22.82%	3.355%
25	17.362	2557	2563	2572	rVB2	480128	1010507	28.87%	4.243%
26	17.545	2589	2594	2601	rVB2	232012	473347	13.52%	1.988%

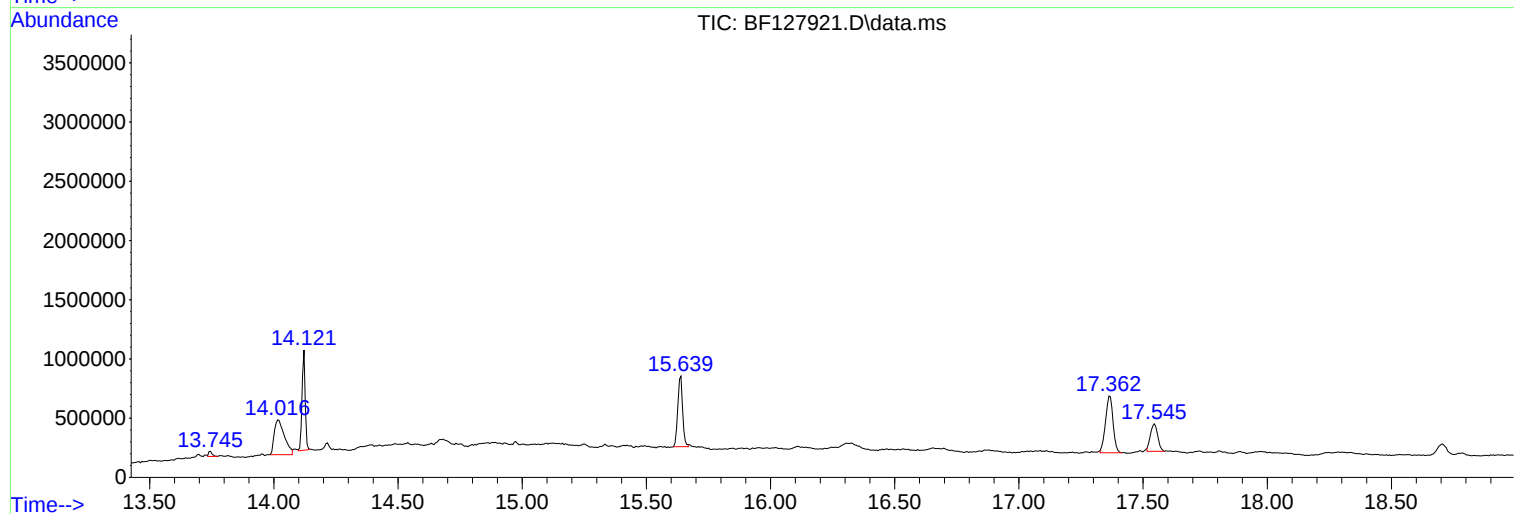
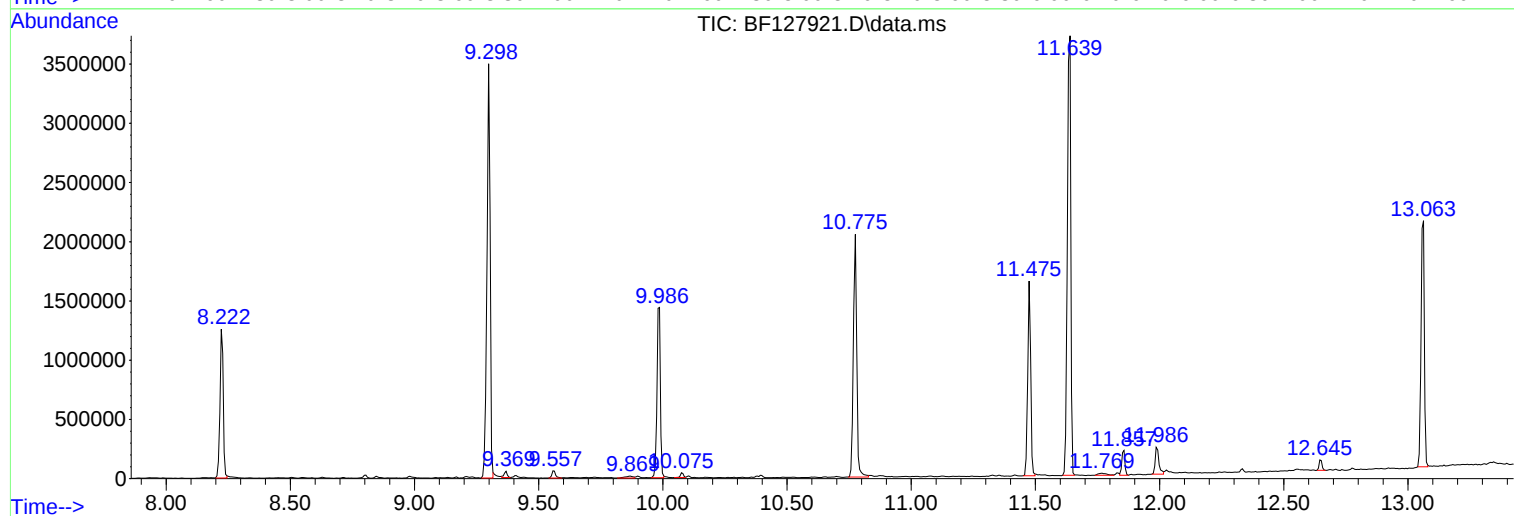
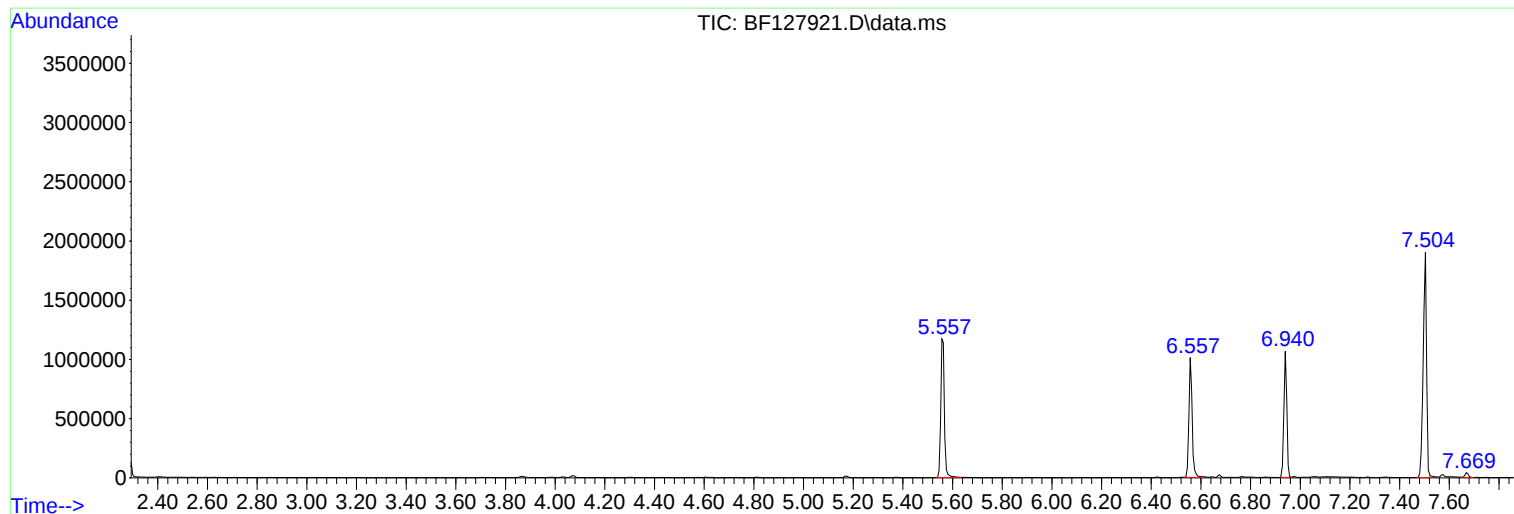
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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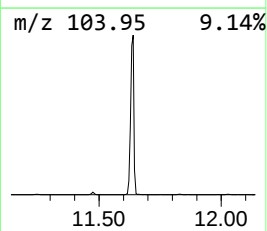
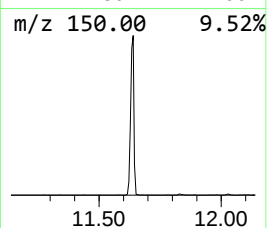
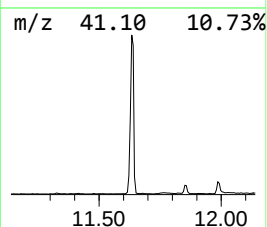
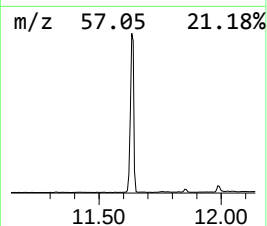
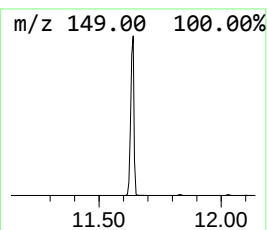
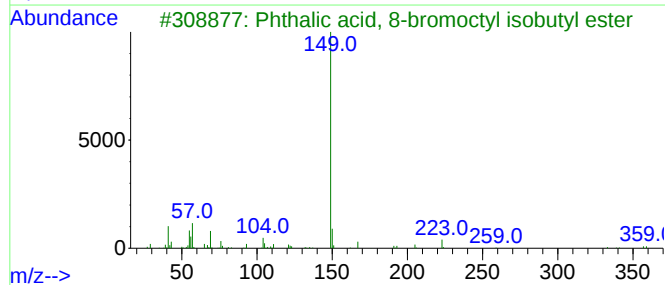
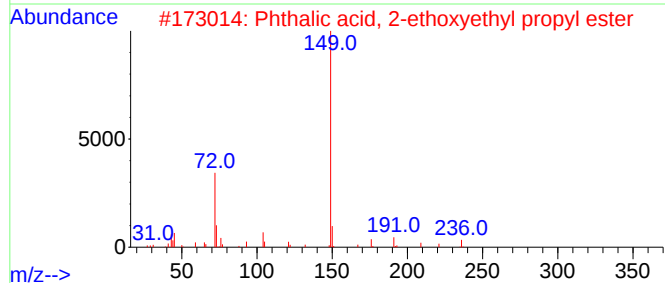
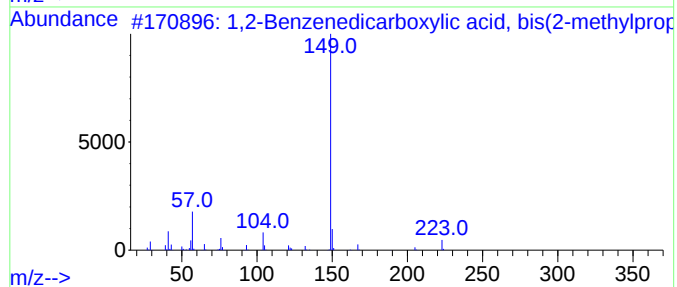
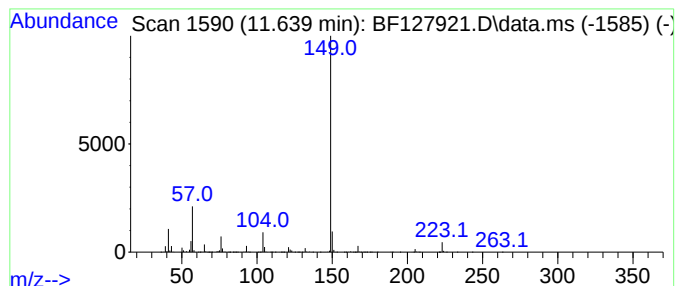
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TIC Integration Parameters: LSCINT.P

Peak Number 1 1,2-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.639	51.40 ng	3500330	Phenanthrene-d10	11.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2			Phthalic acid, 2-ethoxyethyl pro...	280	C15H20O5	1000322-87-0	78
3			Phthalic acid, 8-bromooctyl isobu...	412	C20H29BrO4	1000382-55-3	78
4			Phthalic acid, decyl isobutyl ester	362	C22H34O4	1000308-94-2	78
5			Phthalic acid, cyclohexylmethyl ...	318	C19H26O4	1000309-08-6	78



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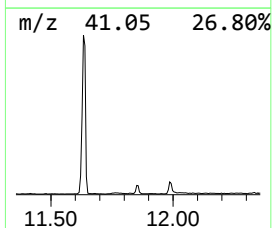
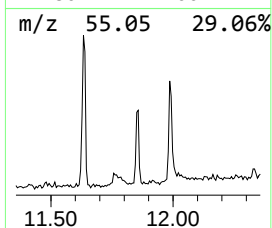
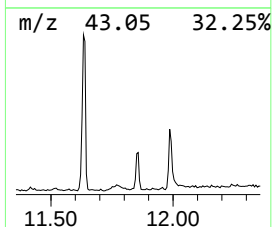
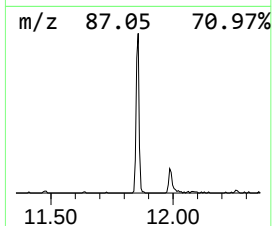
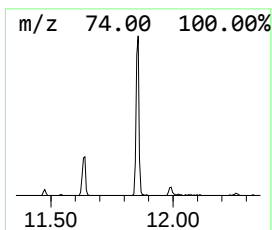
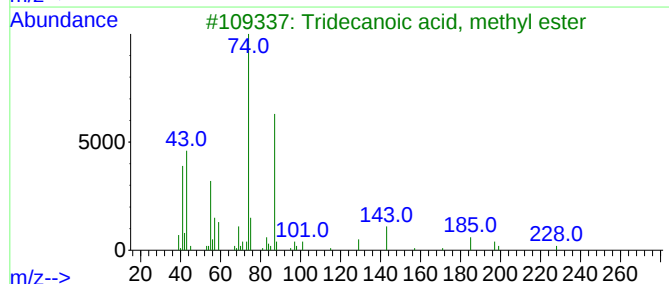
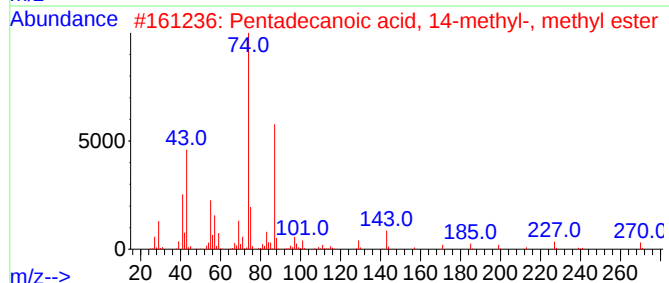
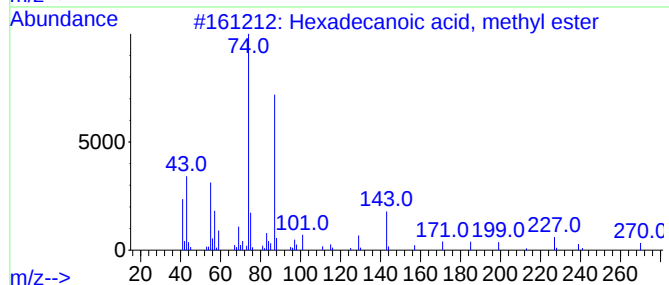
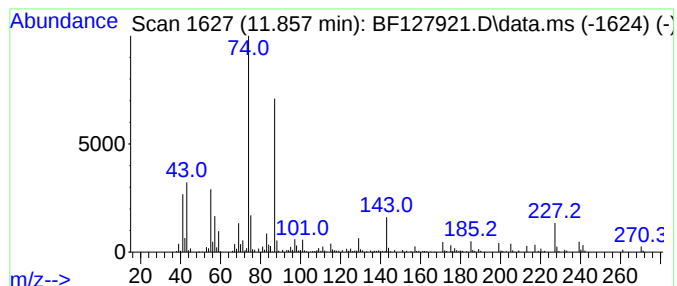
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	2.65 ng	180351	Phenanthrene-d10	11.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
5			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80



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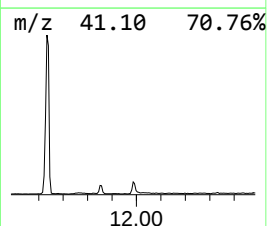
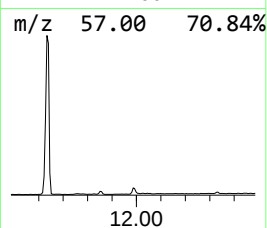
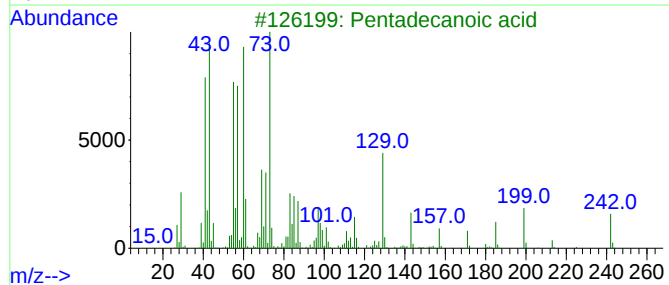
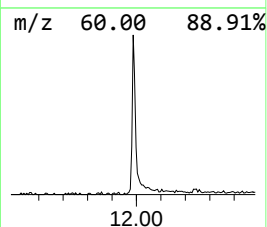
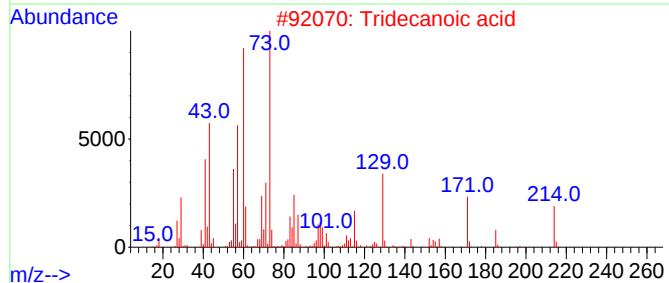
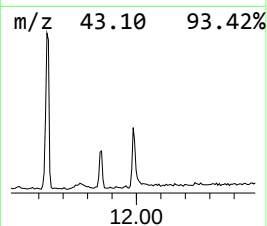
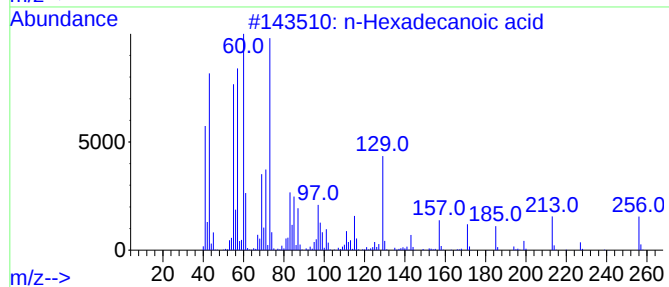
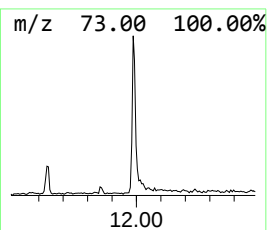
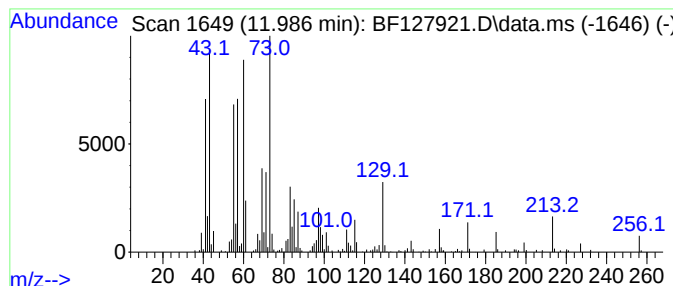
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	3.45 ng	235117	Phenanthrene-d10	11.475

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	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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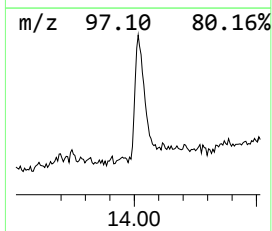
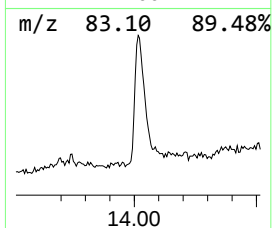
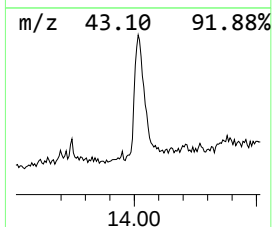
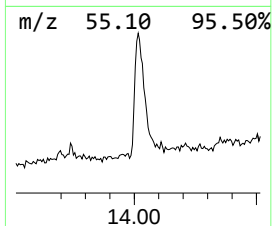
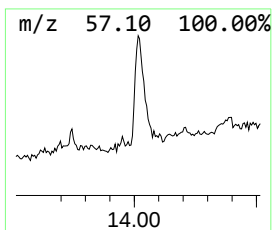
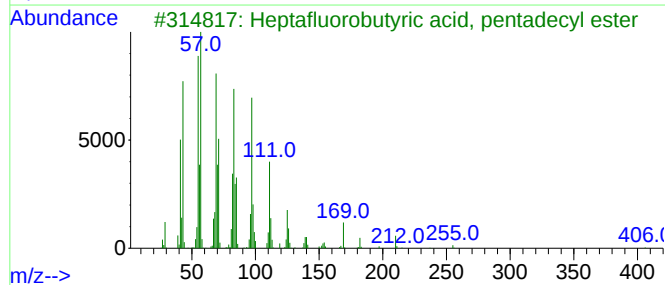
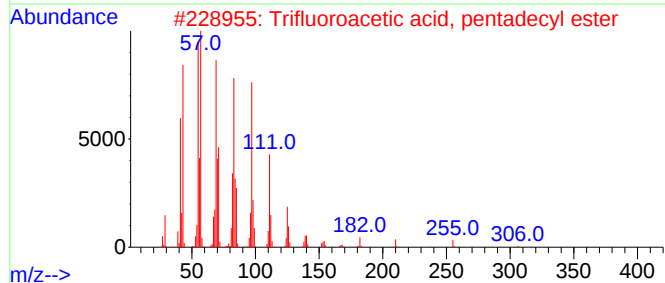
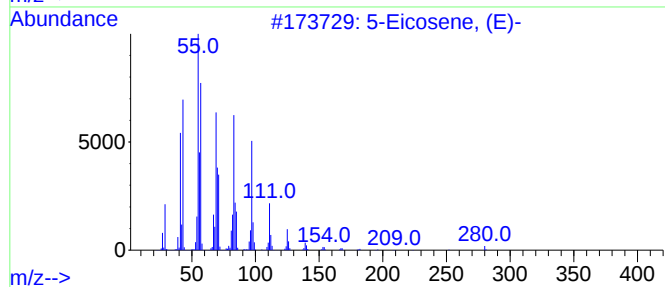
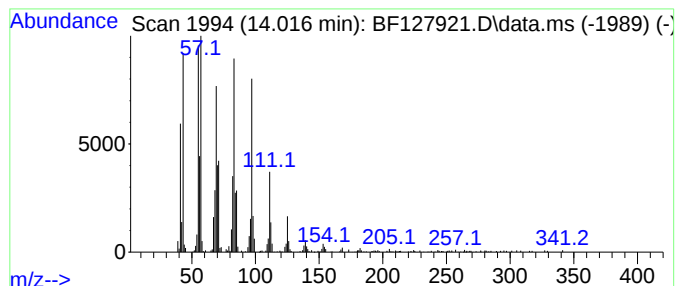
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.016	22.36 ng	832237	Chrysene-d12	14.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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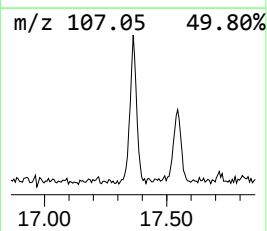
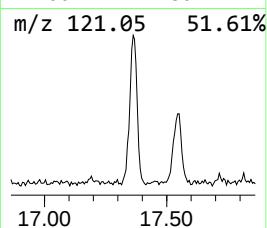
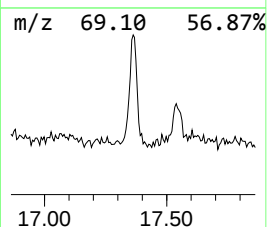
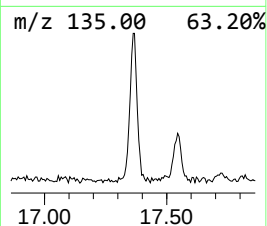
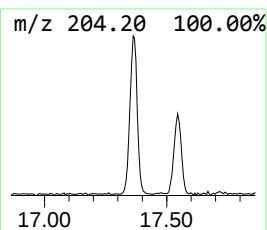
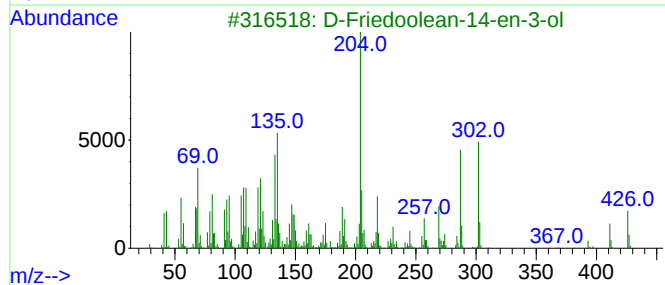
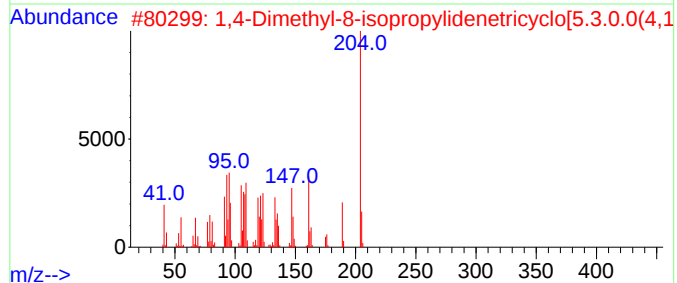
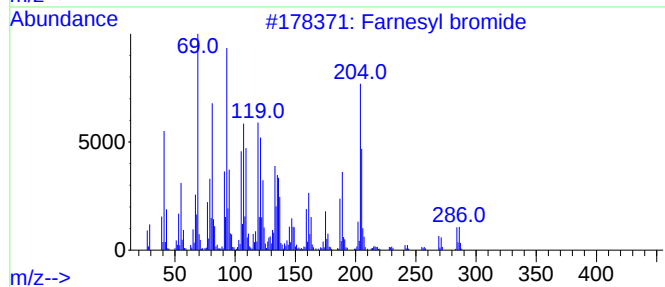
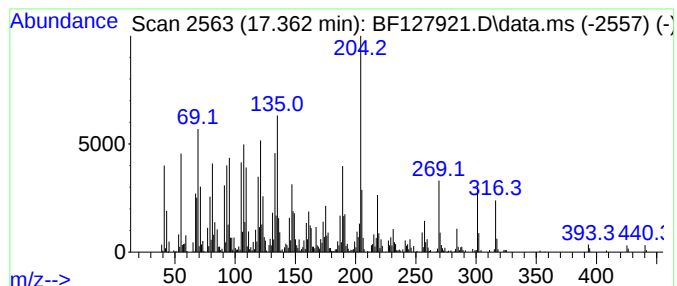
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Peak Number 5 Farnesyl bromide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.362	25.30 ng	1010510	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Farnesyl bromide	284	C15H25Br	006874-67-5	55
2			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	53
3			D-Friedoolean-14-en-3-ol	426	C30H50O	081654-73-1	52
4			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	50
5			1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	49



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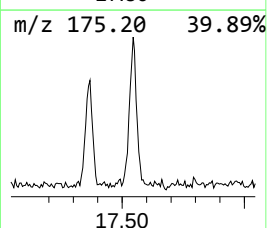
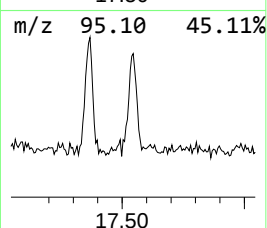
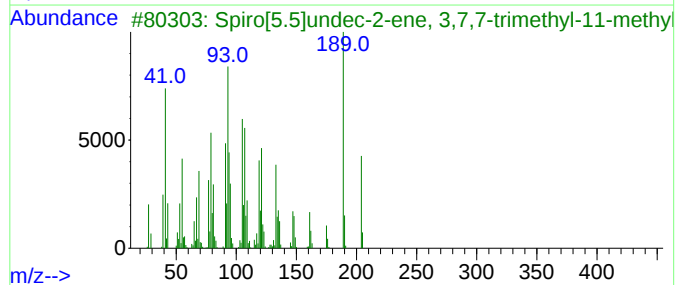
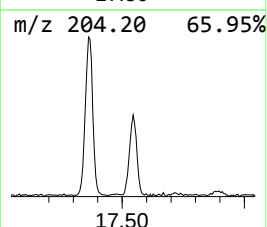
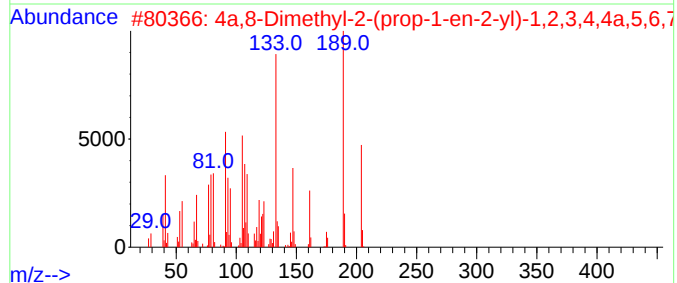
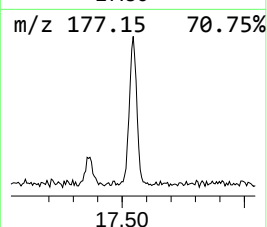
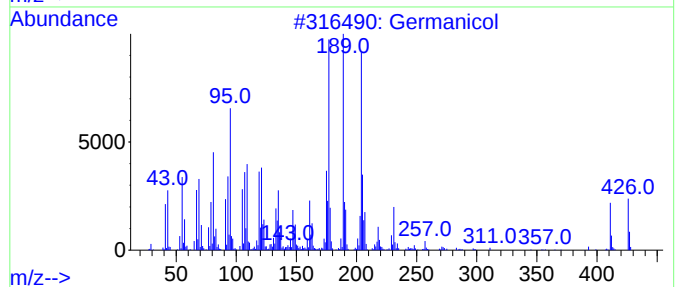
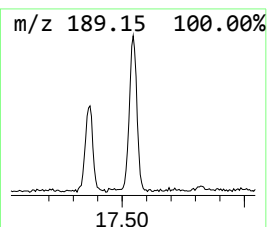
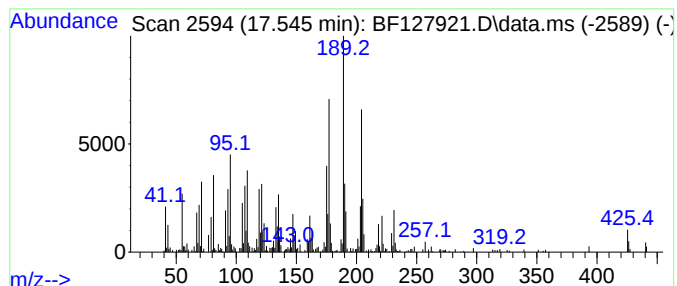
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Germanicol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.545	11.85 ng	473347	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Germanicol	426	C30H50O	000465-02-1	53
2			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	46
3			Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	38
4			(3S,3aR,6R,8aS)-7,7-Dimethyl-8-m...	218	C15H22O	082509-29-3	35
5			3-Acetyl-2,5-dimethylbenzo(b)thi...	204	C12H12OS	006179-04-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127921.D
Acq On : 26 Apr 2022 19:15
Operator : CG\JU
Sample : N2551-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220375-096-21-01-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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
1,2-Benzenedica...	11.639	51.4	ng	3500330	4	11.475	1361920	20.0
Hexadecanoic ac...	11.857	2.6	ng	180351	4	11.475	1361920	20.0
n-Hexadecanoic ...	11.986	3.5	ng	235117	4	11.475	1361920	20.0
5-Eicosene, (E)-	14.016	22.4	ng	832237	5	14.121	744467	20.0
Farnesyl bromide	17.362	25.3	ng	1010510	6	15.639	798918	20.0
Germanicol	17.545	11.9	ng	473347	6	15.639	798918	20.0