

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
 Data File : BF128605.D
 Acq On : 31 May 2022 20:30
 Operator : CG\JU
 Sample : N2952-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P037-SS001-0612-01

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: BF128605.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	468	471	477	rVB	28982	29085	1.25%	0.177%
2	5.504	543	547	560	rBV	2028517	2085375	89.71%	12.687%
3	6.528	717	721	730	rBV	1670057	2015134	86.69%	12.260%
4	6.839	771	774	778	rBV	734648	648183	27.88%	3.944%
5	7.410	865	871	874	rBV	1439600	1415090	60.88%	8.609%
6	8.128	988	993	996	rBV	896597	760136	32.70%	4.625%
7	9.204	1170	1176	1179	rBV	2811061	2324499	100.00%	14.142%
8	9.880	1287	1291	1295	rBV	885995	746954	32.13%	4.544%
9	10.680	1423	1427	1434	rBV	1127799	1084060	46.64%	6.595%
10	10.786	1441	1445	1453	rVB4	30825	62937	2.71%	0.383%
11	11.016	1481	1484	1492	rVB6	19974	32252	1.39%	0.196%
12	11.369	1541	1544	1548	rBV	763329	654482	28.16%	3.982%
13	11.910	1633	1636	1638	rBV2	43302	57603	2.48%	0.350%
14	12.568	1743	1748	1757	rBV2	216788	334171	14.38%	2.033%
15	12.957	1810	1814	1818	rBV	2138429	1889869	81.30%	11.498%
16	13.045	1824	1829	1835	rBV7	26932	70146	3.02%	0.427%
17	13.145	1842	1846	1851	rVB4	27627	49348	2.12%	0.300%
18	13.351	1876	1881	1889	rVB3	167899	273555	11.77%	1.664%
19	13.592	1918	1922	1930	rVB	176539	256408	11.03%	1.560%
20	14.010	1990	1993	1997	rBV	587581	535803	23.05%	3.260%
21	14.057	1997	2001	2006	rVV	147022	217423	9.35%	1.323%
22	14.115	2007	2011	2019	rVB	212897	241317	10.38%	1.468%
23	14.292	2037	2041	2045	rVB	91519	125465	5.40%	0.763%
24	14.721	2110	2114	2120	rVB3	96524	117762	5.07%	0.716%
25	15.486	2239	2244	2248	rBV	319157	409612	17.62%	2.492%

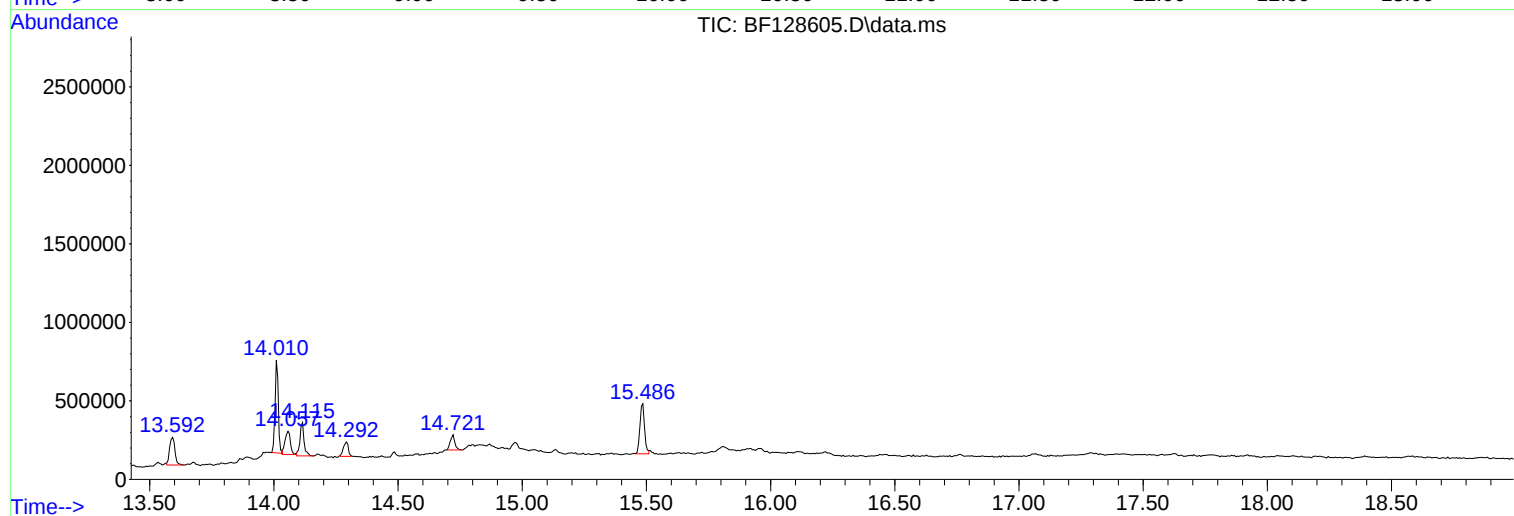
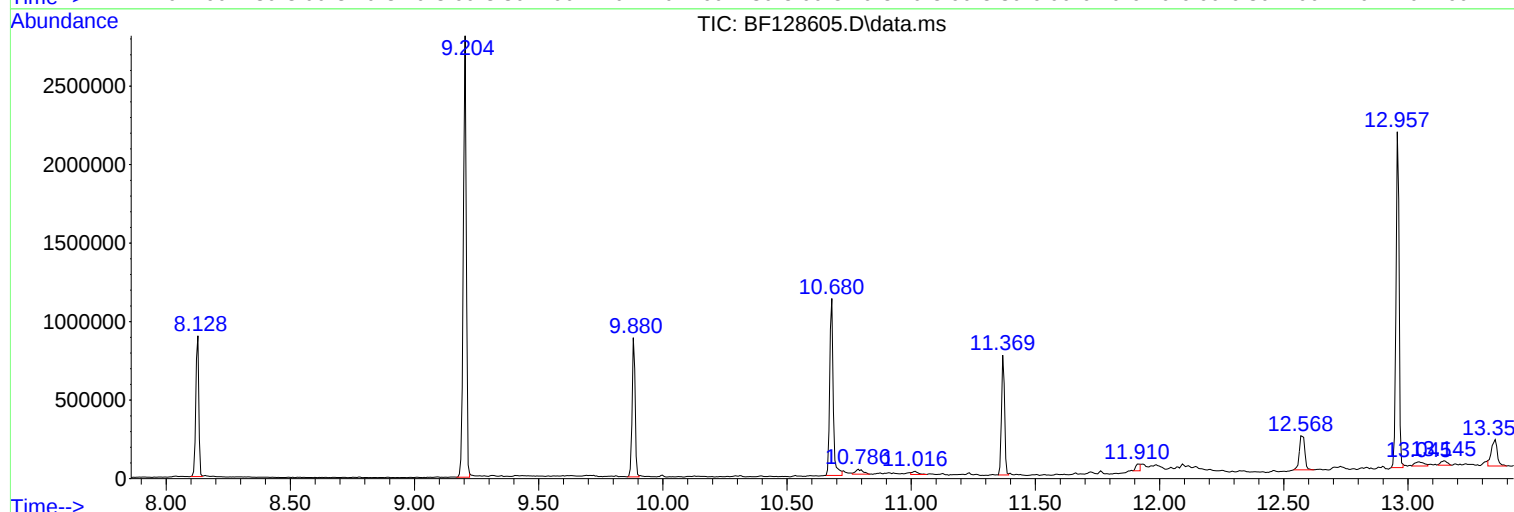
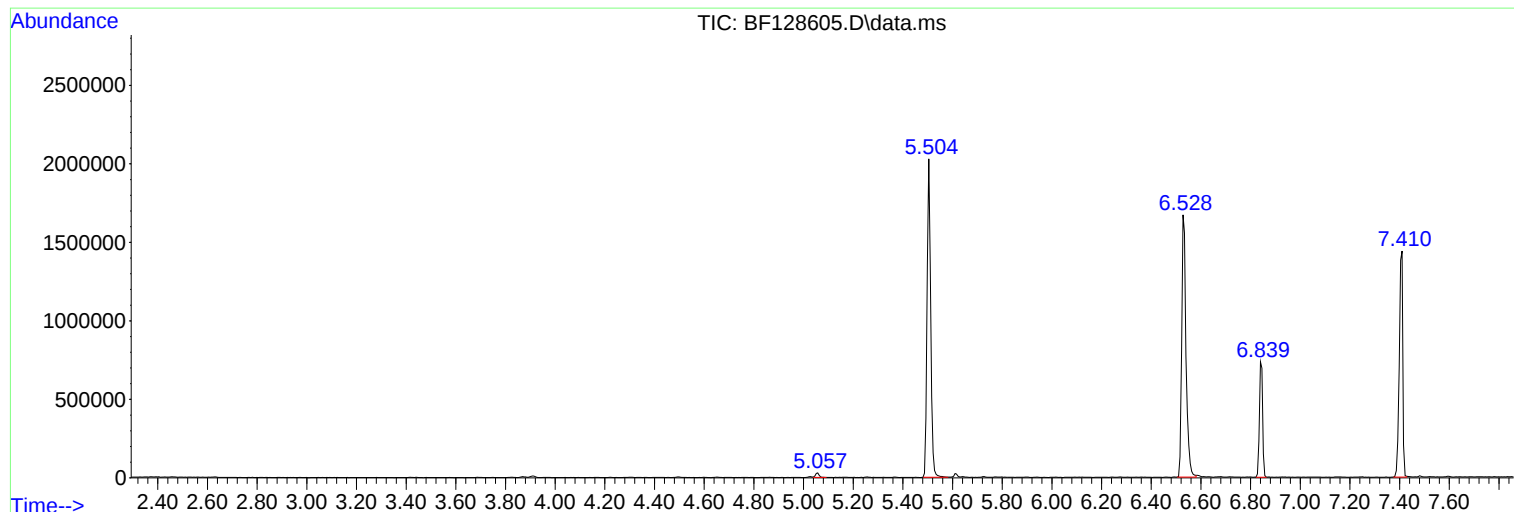
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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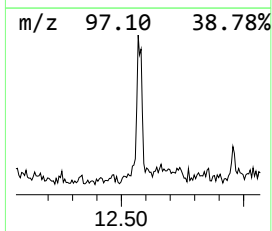
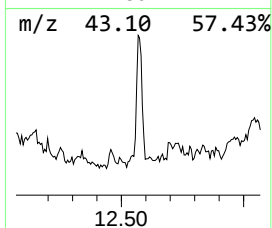
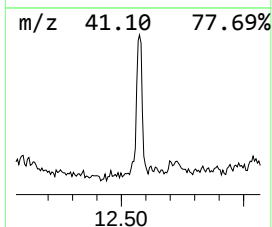
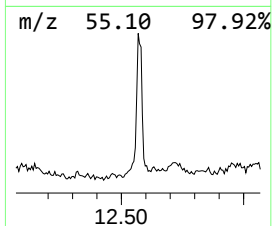
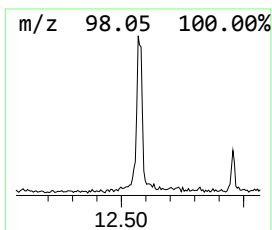
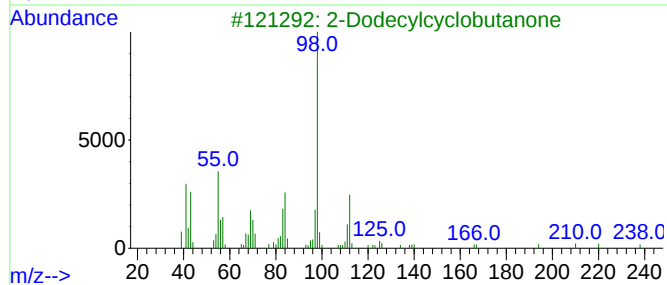
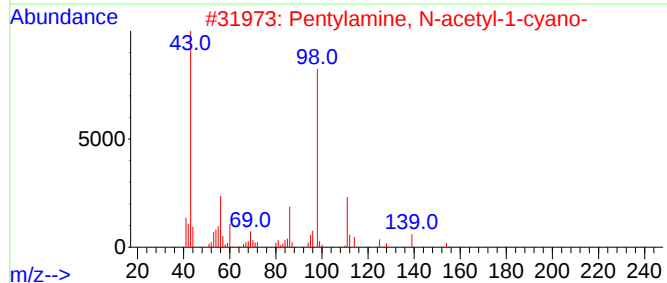
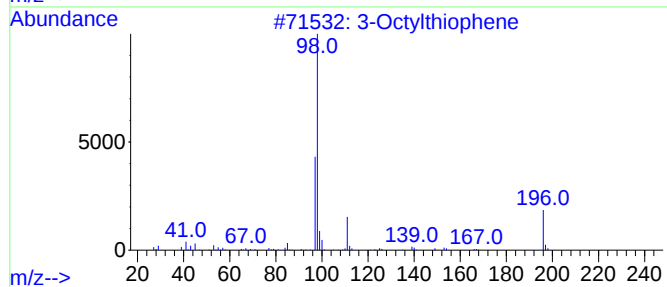
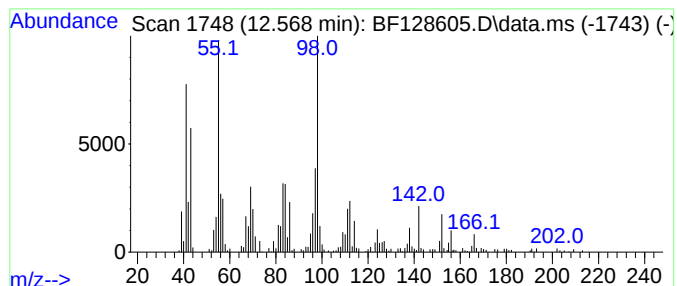
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 unknown12.569 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	10.21 ng	334171	Phenanthrene-d10	11.368

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octylthiophene		196	C12H20S	065016-62-8	38
2	Pentylamine, N-acetyl-1-cyano-		154	C8H14N2O	027395-08-0	38
3	2-Dodecylcyclobutanone		238	C16H30O	035493-46-0	38
4	Undecanoyl chloride		204	C11H21ClO	017746-05-3	38
5	2-(1-Methyl-3-butenyl)cyclohexanone		166	C11H18O	1000424-67-7	30



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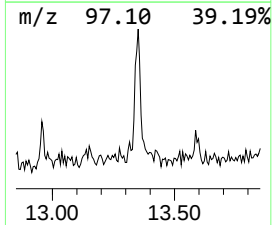
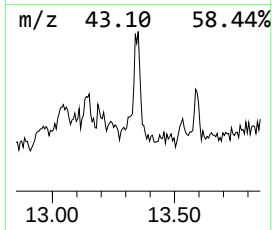
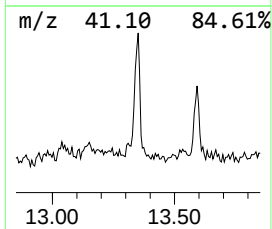
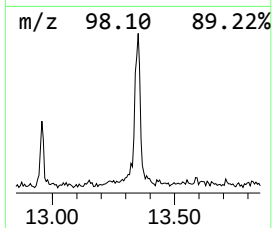
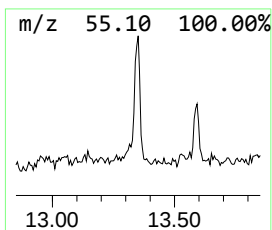
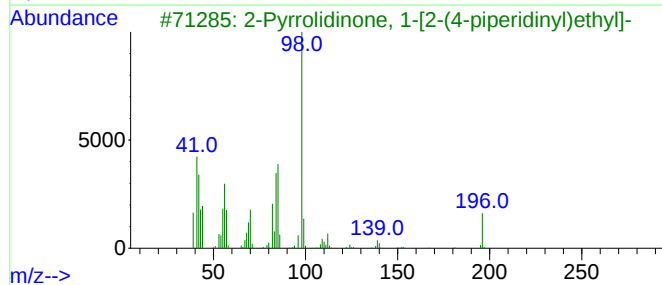
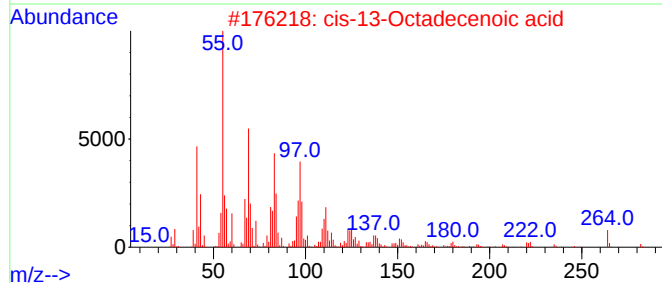
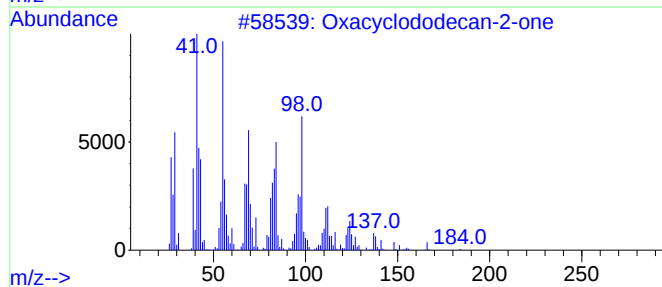
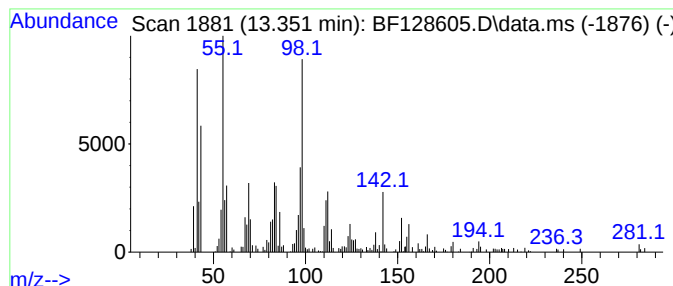
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Peak Number 3 Oxacyclododecan-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.351	10.21 ng	273555	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxacyclododecan-2-one	184	C11H20O2	001725-03-7	53
2			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	47
3			2-Pyrrolidinone, 1-[2-(4-piperid...	196	C11H20N2O	1000338-00-9	35
4			3-Methyl-1-cyclohexanecarboxylic...	142	C8H14O2	1000453-56-9	35
5			Cyclononane	140	C9H16O	003350-30-9	30



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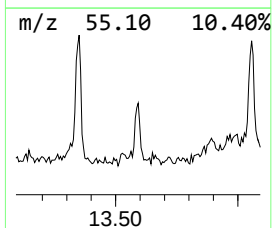
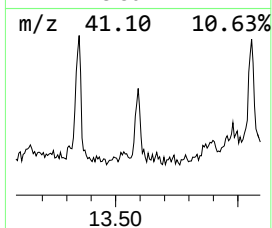
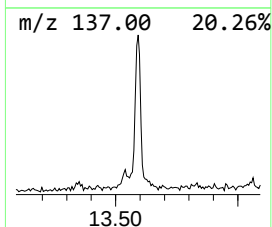
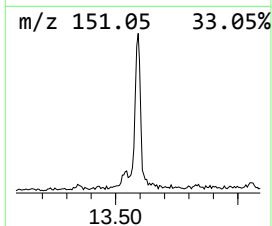
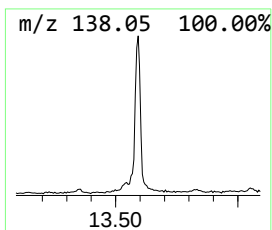
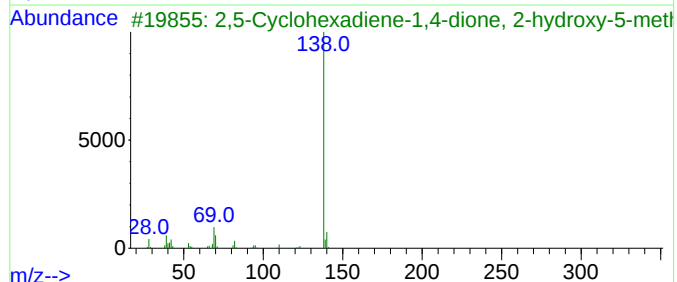
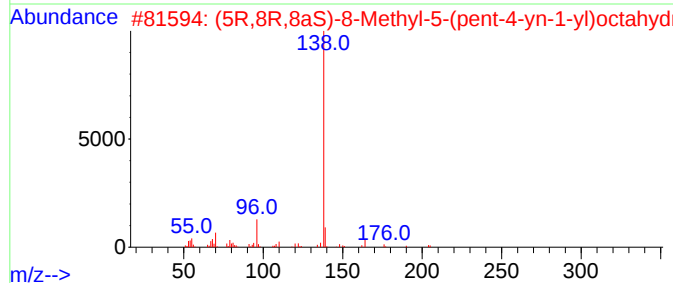
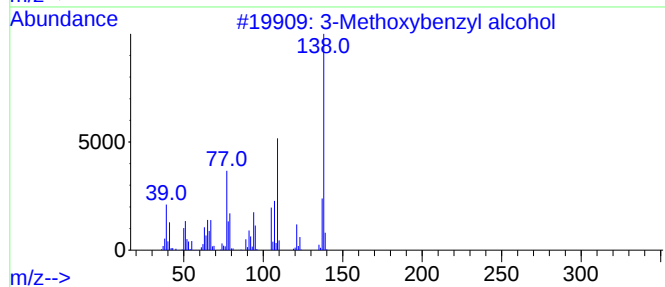
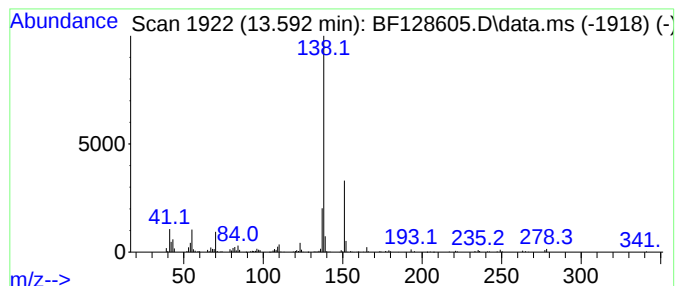
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 3-Methoxybenzyl alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.592	9.57 ng	256408	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methoxybenzyl alcohol	138	C8H10O2	006971-51-3	53
2			(5R,8R,8aS)-8-Methyl-5-(pent-4-y...	205	C14H23N	109175-46-4	50
3			2,5-Cyclohexadiene-1,4-dione, 2-...	138	C7H6O3	000615-91-8	50
4			(Z)-7-((5R,8R,8aS)-8-Methyloctah...	251	C16H29NO	1000367-21-5	50
5			(5R,8R)-8-Methyl-5-pentyloctahyd...	209	C14H27N	117959-79-2	50



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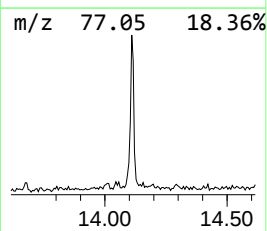
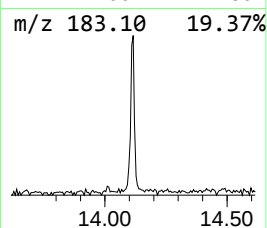
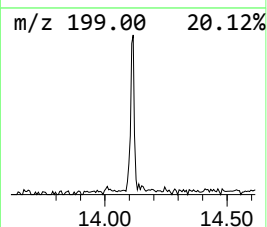
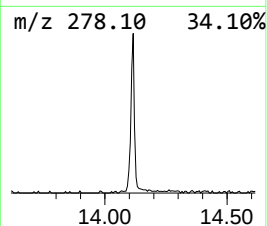
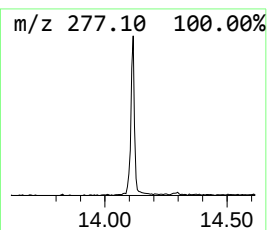
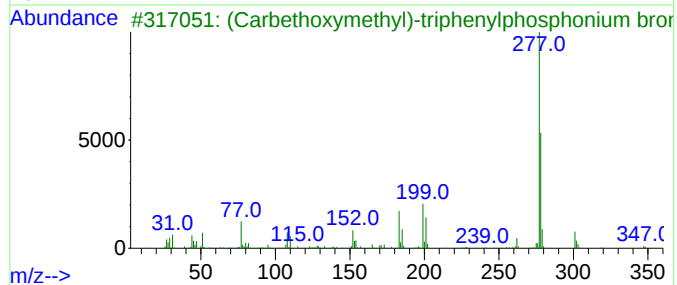
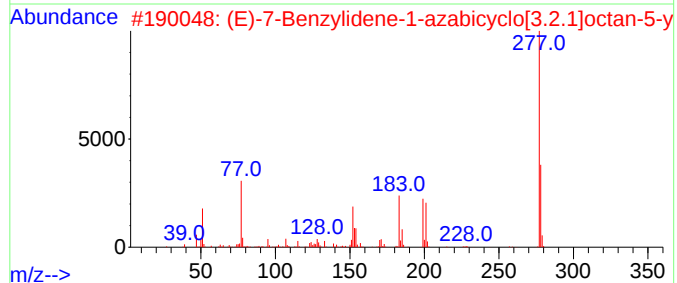
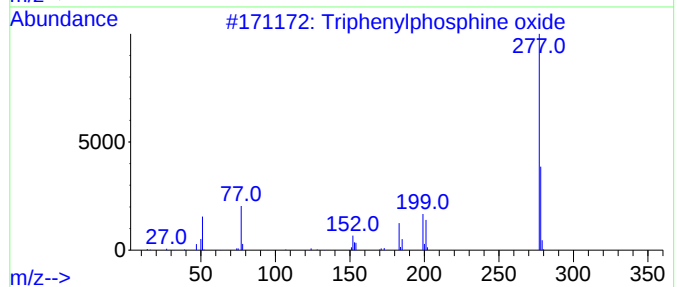
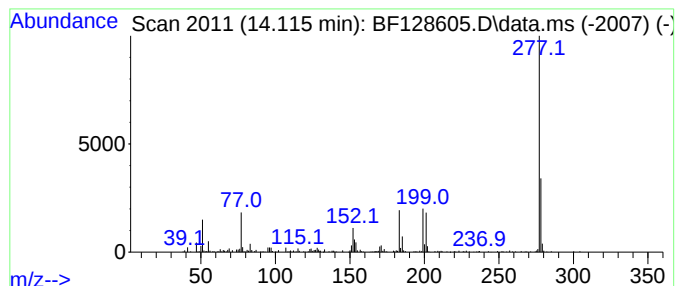
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.115	9.01 ng	241317	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	49
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	37
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	28
5			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	28



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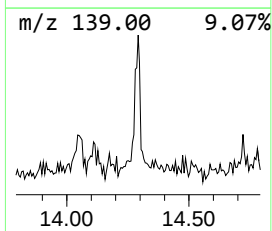
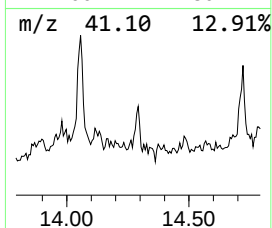
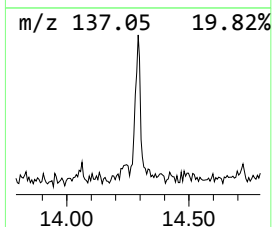
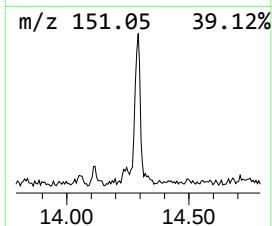
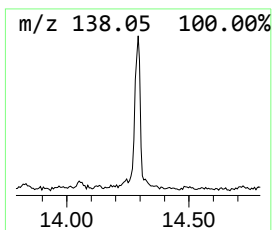
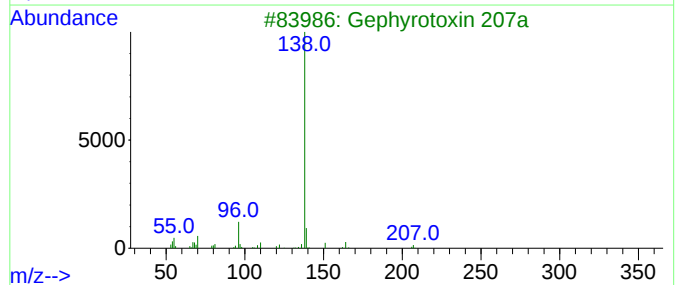
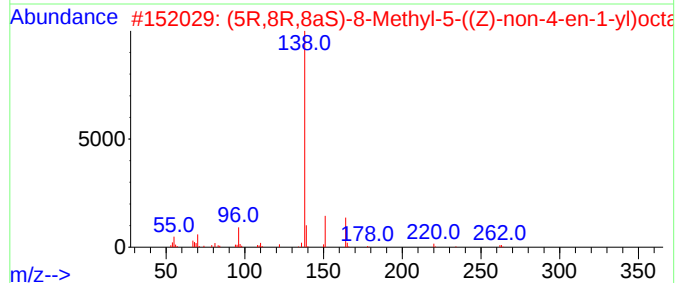
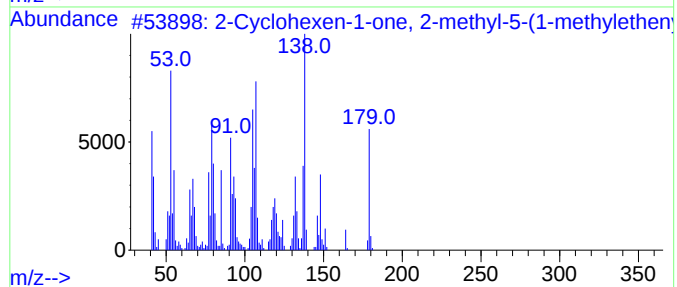
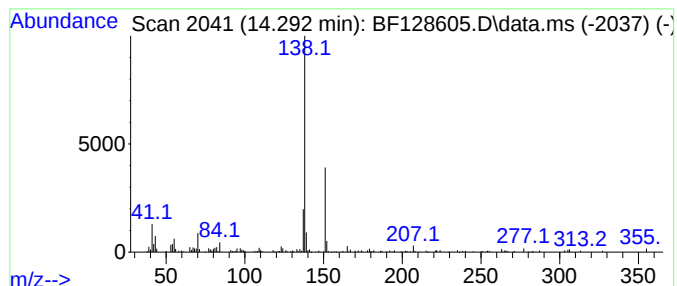
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Peak Number 6 2-Cyclohexen-1-one, 2-methy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.292	4.68 ng	125465	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one, 2-methyl-5-(...	179	C11H17NO	057397-12-3	60
2			(5R,8R,8aS)-8-Methyl-5-((Z)-non-...	263	C18H33N	1000367-14-0	47
3			Gephyrotoxin 207a	207	C14H25N	141724-48-3	43
4			Succinic acid, 2,2,3,3-tetraflu...	352	C15H16F4O5	1000390-95-1	43
5			(5R,8R)-8-Methyl-5-pentyloctahyd...	209	C14H27N	117959-79-2	43



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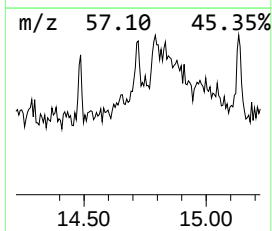
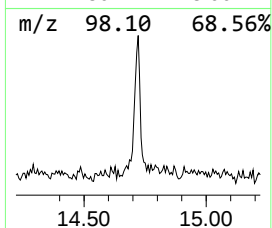
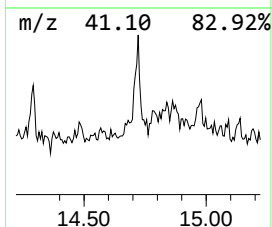
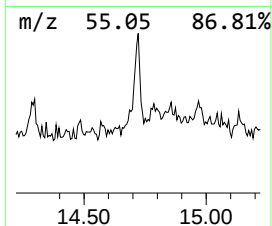
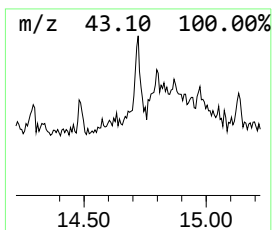
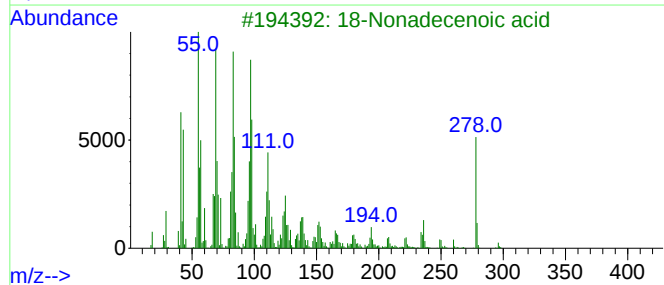
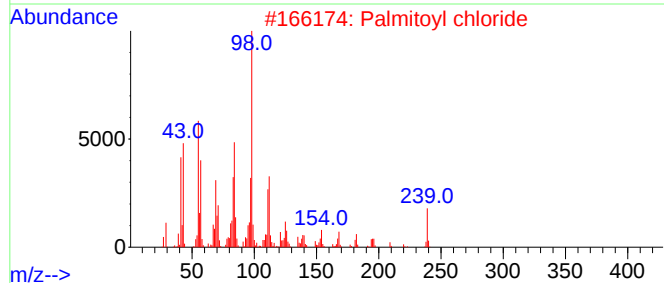
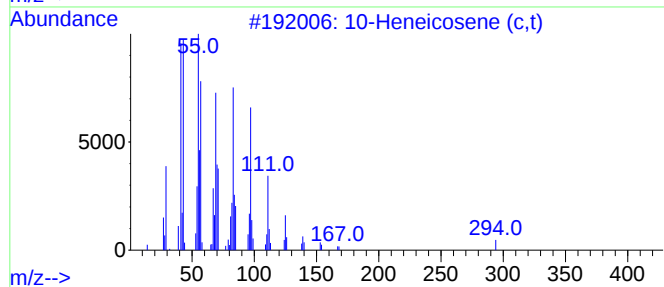
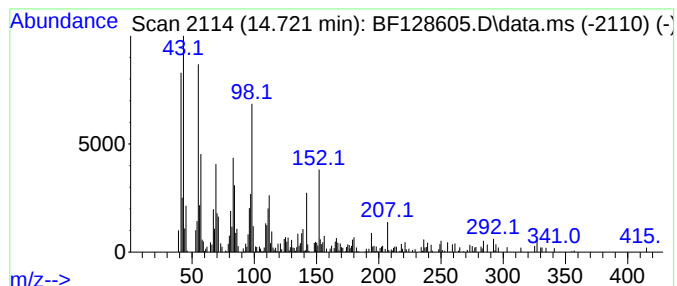
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 10-Heneicosene (c,t) Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	4.40 ng	117762	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Heneicosene (c,t)	294	C21H42	095008-11-0	56
2			Palmitoyl chloride	274	C16H31ClO	000112-67-4	49
3			18-Nonadecenoic acid	296	C19H36O2	076998-87-3	49
4			Cyclooctanone	126	C8H14O	000502-49-8	46
5			Oxacyclotridecan-2-one	198	C12H22O2	000947-05-7	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128605.D
Acq On : 31 May 2022 20:30
Operator : CG\JU
Sample : N2952-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P037-SS001-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
unknown12.569	12.569	10.2	ng	334171	4	11.368	654482	20.0
2-[2-[2-[2-[2-[...	13.045	2.6	ng	70146	5	14.009	535803	20.0
Oxacyclododecan...	13.351	10.2	ng	273555	5	14.009	535803	20.0
3-Methoxybenzyl...	13.592	9.6	ng	256408	5	14.009	535803	20.0
Triphenylphosph...	14.115	9.0	ng	241317	5	14.009	535803	20.0
2-Cyclohexen-1-...	14.292	4.7	ng	125465	5	14.009	535803	20.0
10-Heneicosene ...	14.721	4.4	ng	117762	5	14.009	535803	20.0