

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
 Data File : BF126308.D
 Acq On : 21 Dec 2021 21:18
 Operator : JU/CG
 Sample : M5184-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126308.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	17	rVB	319820	371376	6.54%	0.989%
2	5.428	563	568	571	rBV	2787708	2553918	44.97%	6.799%
3	6.434	735	739	758	rBV	1210677	1759898	30.99%	4.685%
4	6.816	800	804	807	rBV	1381183	1148699	20.23%	3.058%
5	6.957	824	828	842	rBV	1207660	1262472	22.23%	3.361%
6	7.381	893	900	903	rBV	3514590	3972991	69.96%	10.578%
7	8.098	1017	1022	1033	rBV	1748248	1651943	29.09%	4.398%
8	9.180	1199	1206	1209	rBV	5078155	5679121	100.00%	15.120%
9	9.263	1217	1220	1225	rVB2	72141	80299	1.41%	0.214%
10	9.851	1315	1320	1332	rVV	1728484	1846661	32.52%	4.916%
11	10.645	1449	1455	1458	rBV	3203685	3491107	61.47%	9.295%
12	11.339	1569	1573	1579	rBV	1795708	1659040	29.21%	4.417%
13	11.504	1596	1601	1607	rVB2	51081	66252	1.17%	0.176%
14	11.557	1607	1610	1614	rBV	138852	116872	2.06%	0.311%
15	11.733	1635	1640	1643	rBV	2065272	1841060	32.42%	4.902%
16	11.869	1660	1663	1666	rBV	102350	99420	1.75%	0.265%
17	11.916	1666	1671	1674	rVV2	475934	459176	8.09%	1.222%
18	12.374	1746	1749	1754	rVB	72282	69404	1.22%	0.185%
19	12.927	1838	1843	1846	rBV	4353037	4842753	85.27%	12.893%
20	13.574	1950	1953	1957	rVB	70510	66131	1.16%	0.176%
21	13.933	2009	2014	2017	rBV3	104141	195758	3.45%	0.521%
22	13.974	2017	2021	2032	rVV	1297227	1476920	26.01%	3.932%
23	14.068	2032	2037	2049	rVB	283846	382675	6.74%	1.019%
24	14.610	2125	2129	2133	rVB	837398	775037	13.65%	2.063%
25	14.657	2134	2137	2141	rVV2	49608	56794	1.00%	0.151%
26	14.739	2147	2151	2152	rBV2	152078	181759	3.20%	0.484%
27	14.839	2164	2168	2172	rBV	85241	116725	2.06%	0.311%
28	14.880	2172	2175	2179	rVB	52630	61563	1.08%	0.164%
29	14.933	2179	2184	2188	rBV	97844	114929	2.02%	0.306%
30	15.027	2196	2200	2204	rBV	65983	69985	1.23%	0.186%
31	15.421	2261	2267	2288	rBV	655765	1089927	19.19%	2.902%

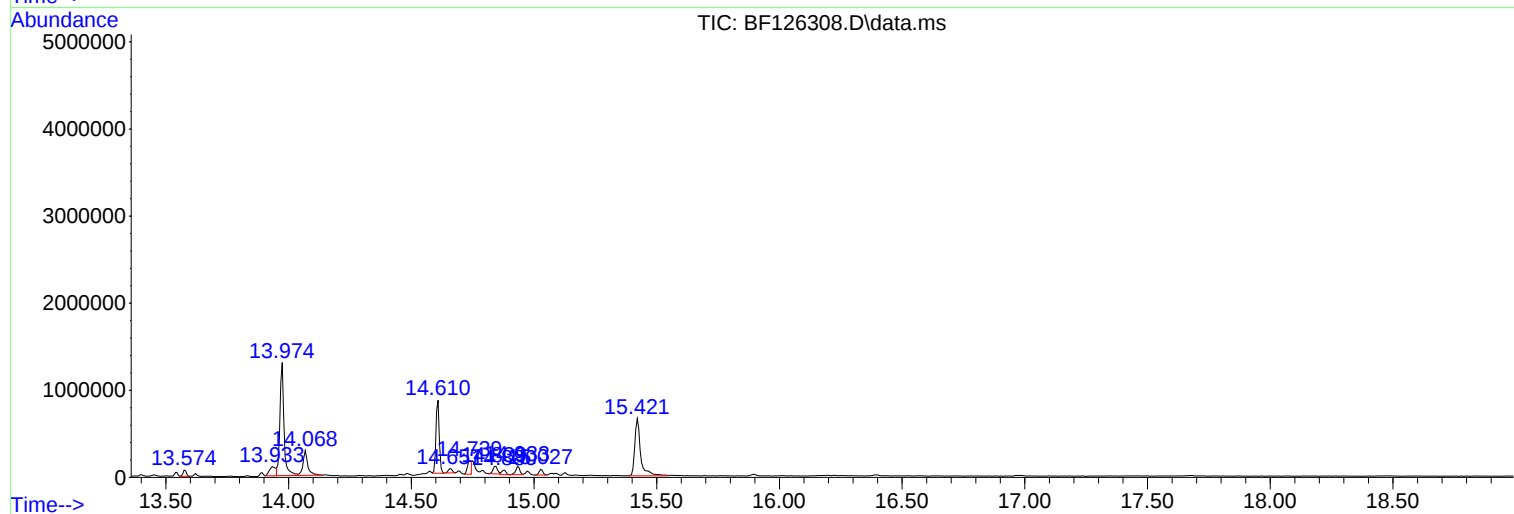
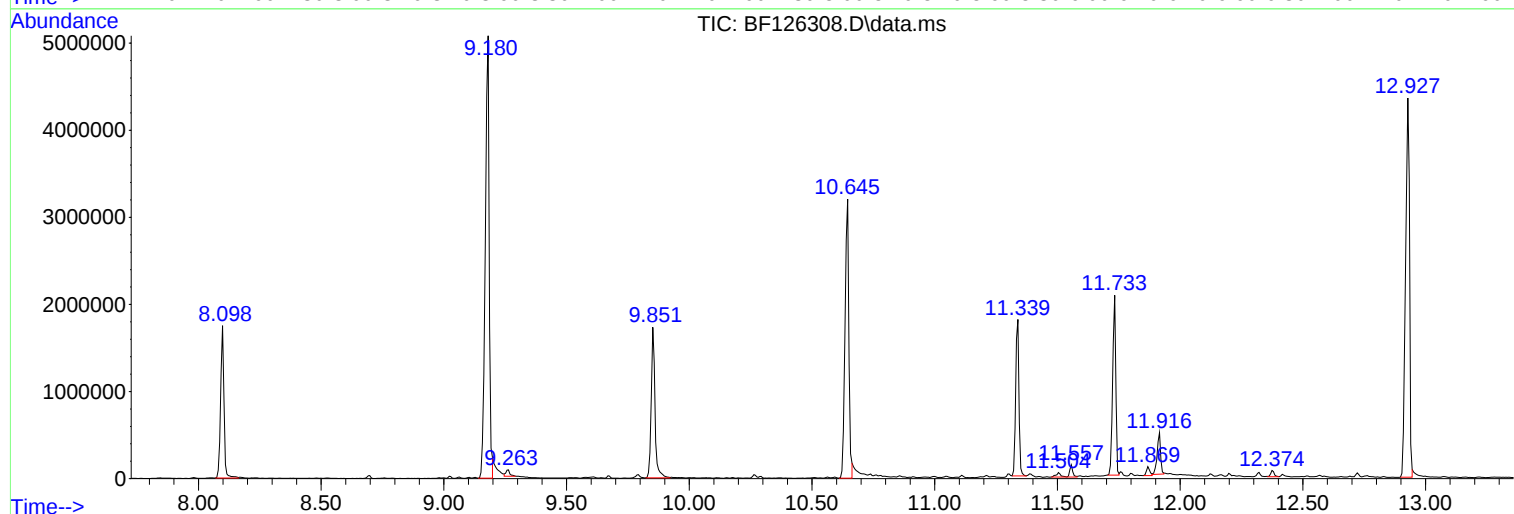
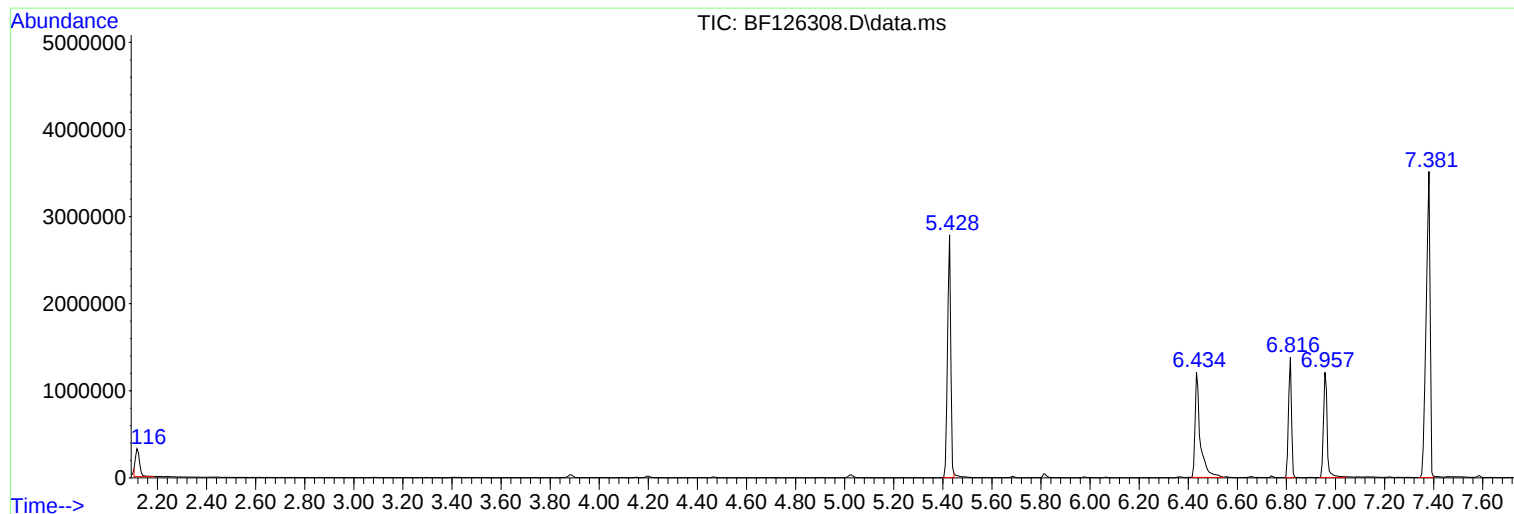
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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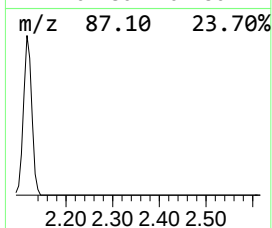
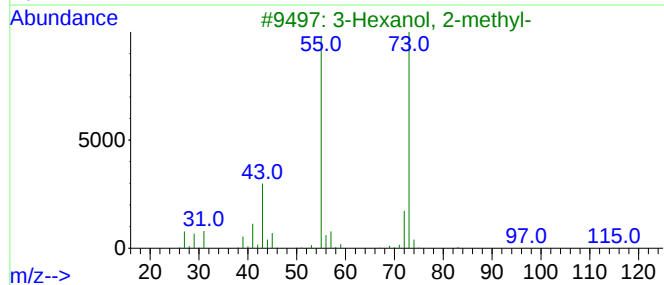
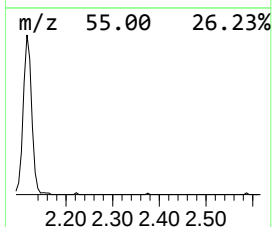
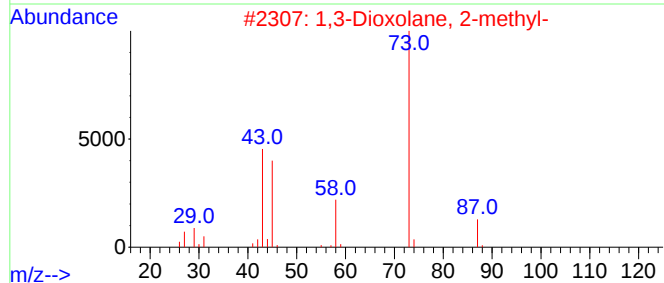
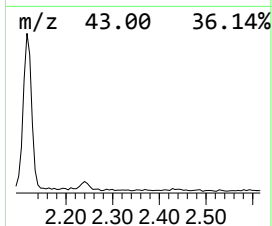
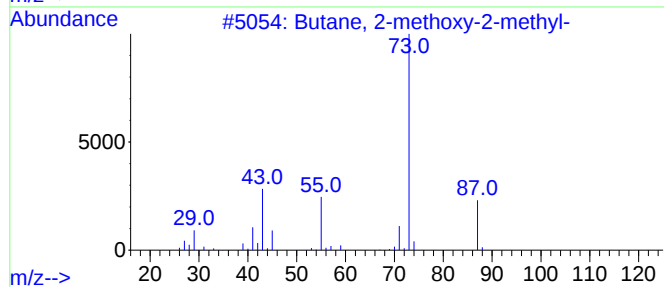
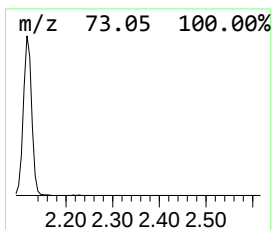
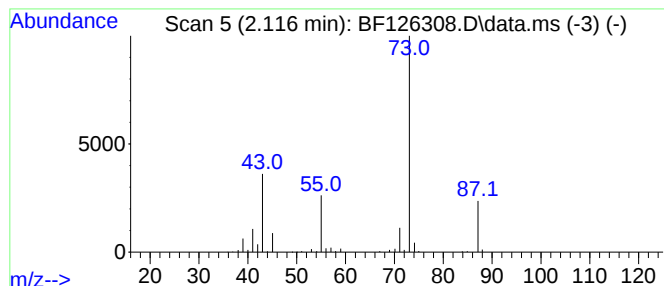
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	6.47 ng	371376	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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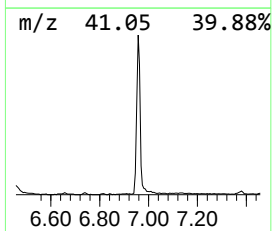
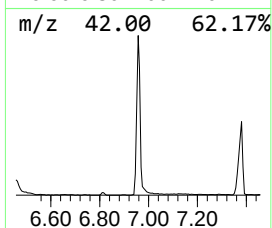
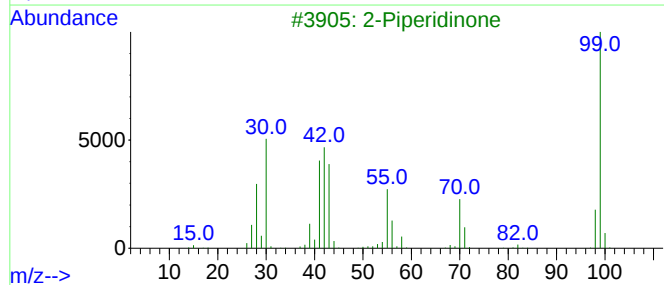
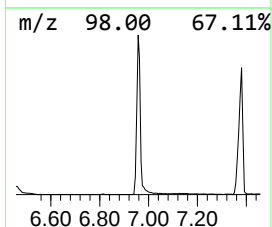
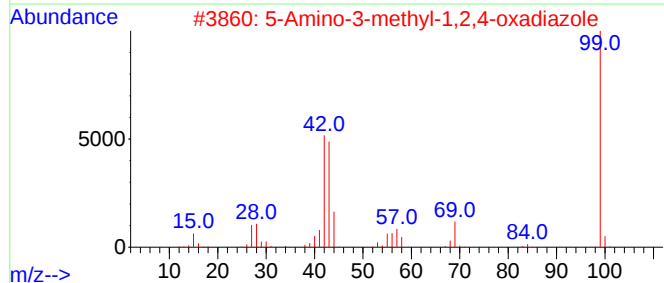
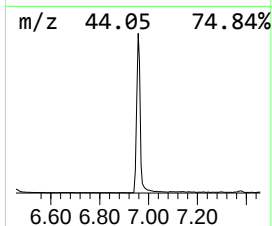
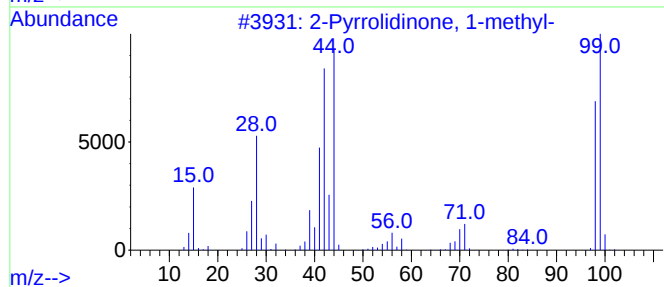
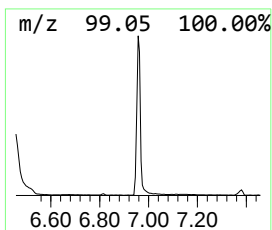
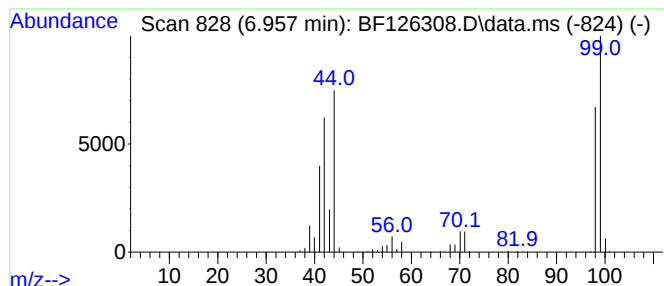
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Peak Number 2 2-Pyrrolidinone, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.957	21.98 ng	1262470	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	94
2			5-Amino-3-methyl-1,2,4-oxadiazole	99	C3H5N3O	003663-39-6	38
3			2-Piperidinone	99	C5H9NO	000675-20-7	25
4			5-Aminopentanamide	116	C5H12N2O	013023-70-6	25
5			1,3,2-Dioxaborolane, 2,4-diethyl-	128	C6H13BO2	057633-63-3	23



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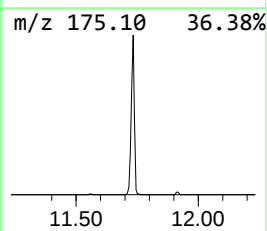
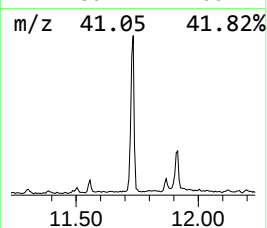
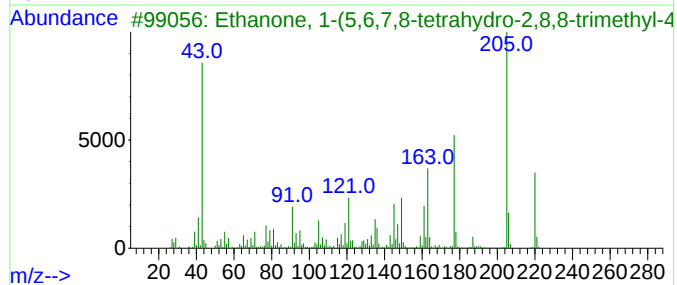
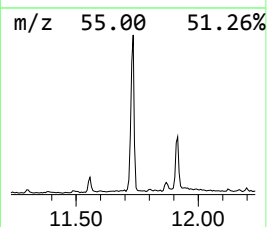
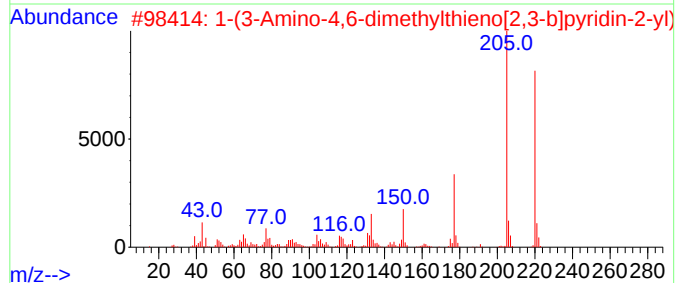
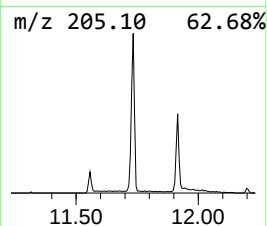
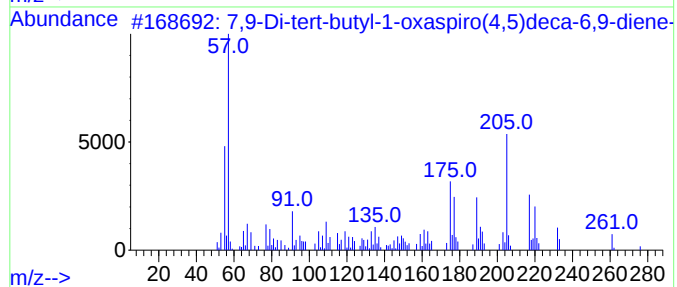
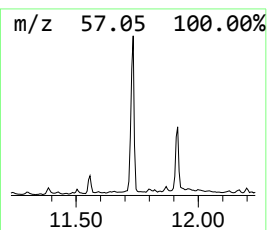
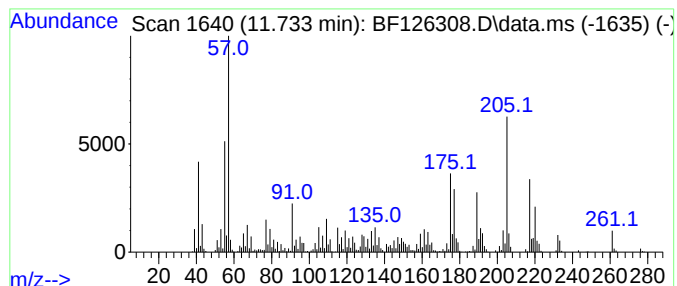
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Peak Number 3 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.733	22.19 ng	1841060	Phenanthrene-d10	11.339	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	98
2	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45
3	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	41
4	9-Acetylphenanthrene	220	C16H12O	002039-77-2	38
5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	30



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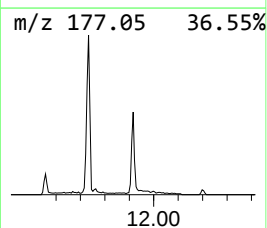
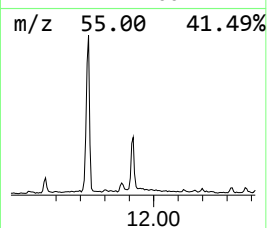
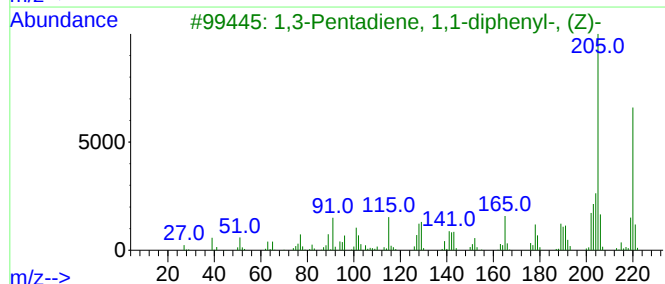
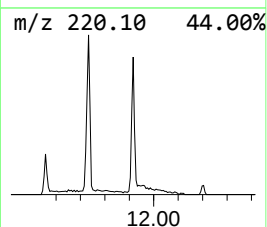
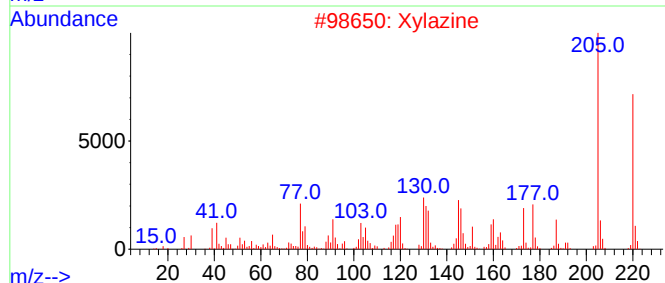
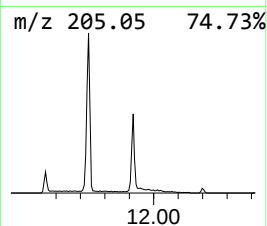
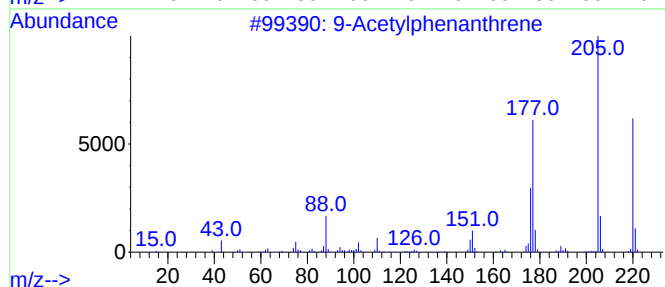
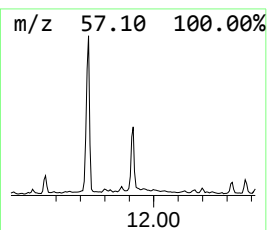
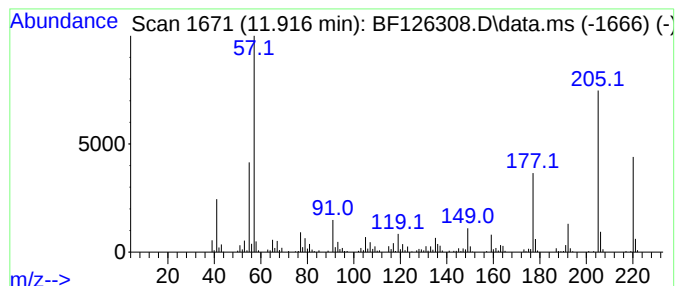
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Peak Number 4 9-Acetylphenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	5.54 ng	459176	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Acetylphenanthrene	220	C16H12O	002039-77-2	76
2			Xylazine	220	C12H16N2S	007361-61-7	58
3			1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	53
4			2-(3,3-Dimethylbut-1-ynyl)thieno...	220	C12H12S2	1010250-48-5	50
5			(4,6-Dimethyl-2-pyrimidinyl)cyan...	220	C10H16N4Si	1000485-05-4	50



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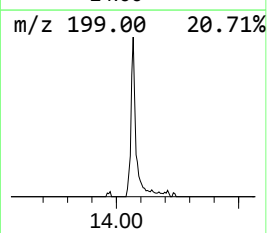
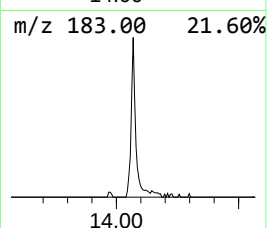
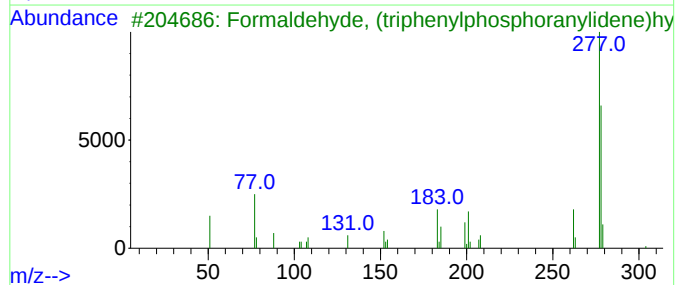
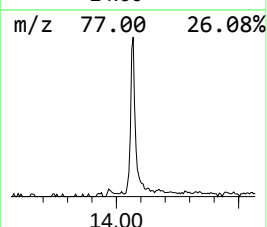
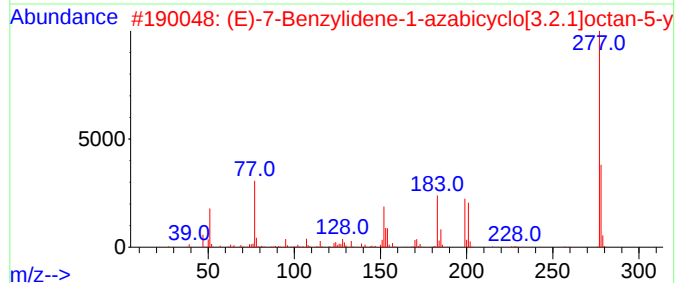
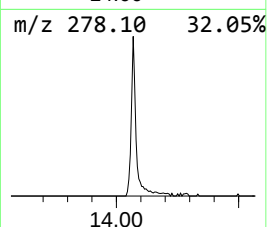
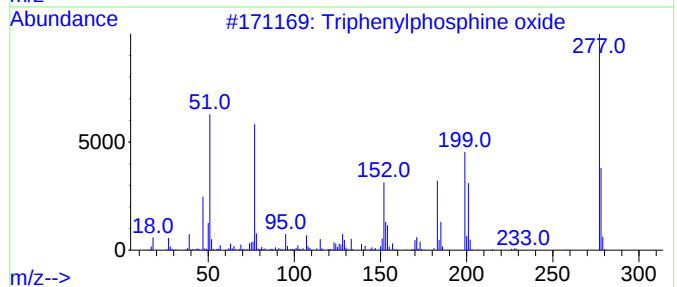
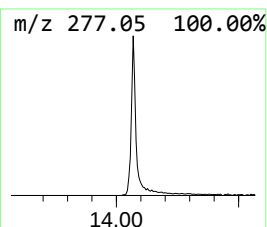
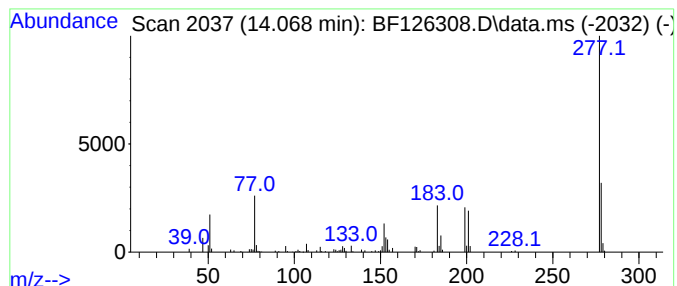
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.068	5.18 ng	382675	Chrysene-d12	13.974

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	81
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	25



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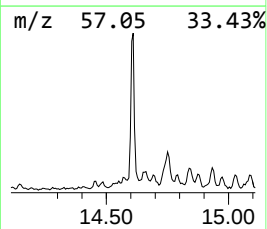
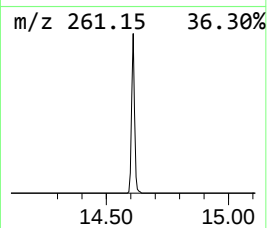
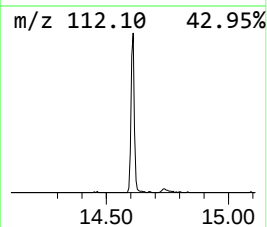
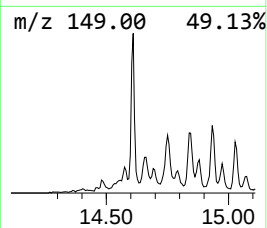
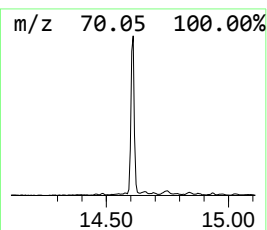
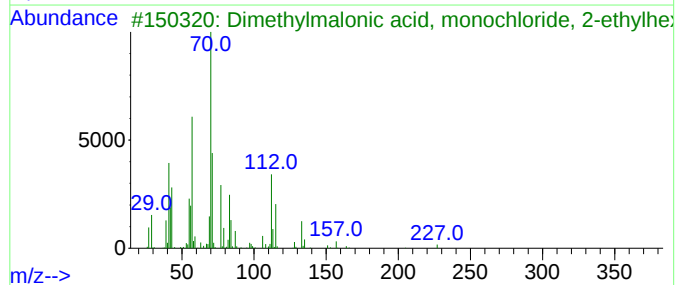
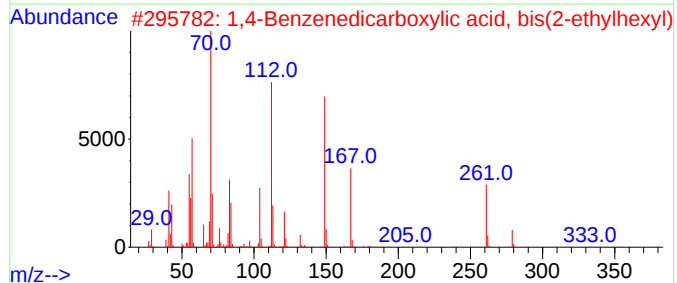
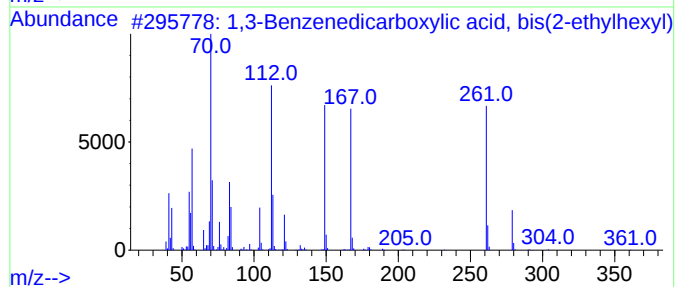
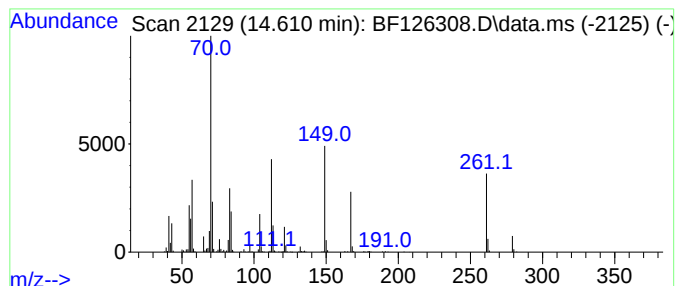
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,3-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.610	10.50 ng	775037	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52
3			Dimethylmalonic acid, monochlori...	262	C13H23ClO3	1000361-64-8	37
4			Cyclohexanamine, N-methyl-	113	C7H15N	000100-60-7	25
5			Methyl 1-acetylpyrrolidine-2-car...	171	C8H13NO3	018800-83-4	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126308.D
Acq On : 21 Dec 2021 21:18
Operator : JU/CG
Sample : M5184-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3

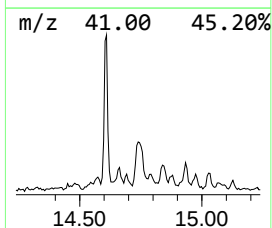
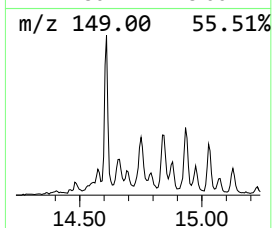
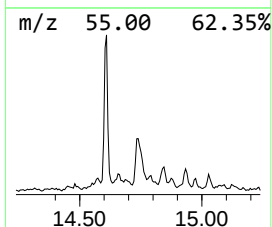
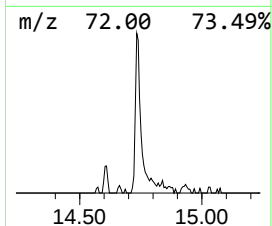
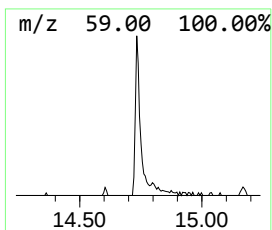
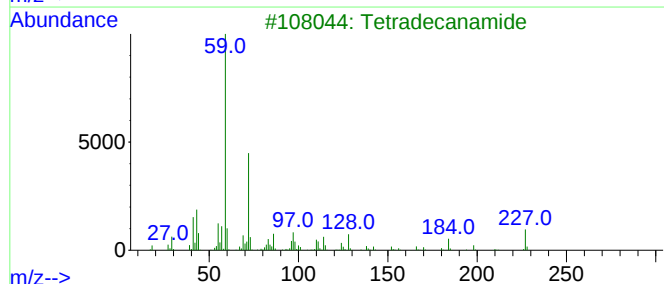
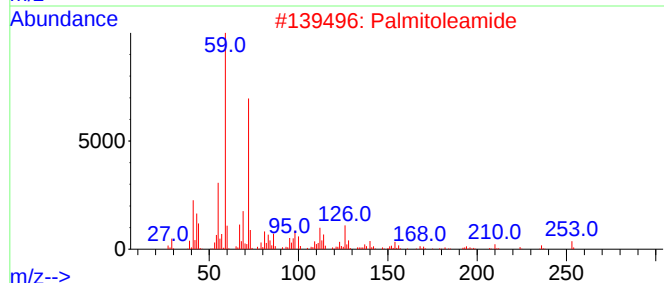
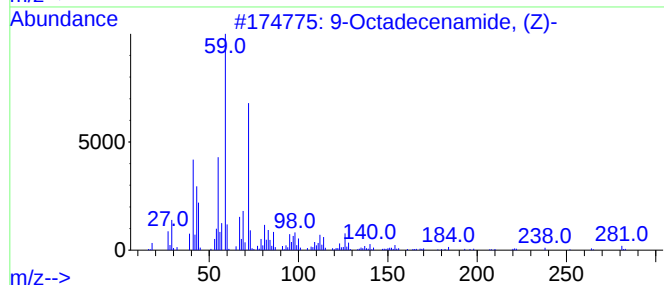
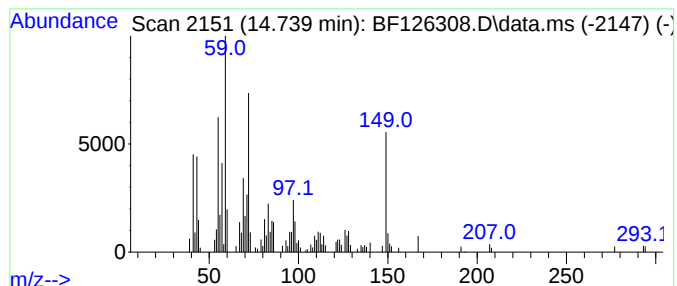
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.739	3.34 ng	181759	Perylene-d12	15.421

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
2		Palmitoleamide	253	C16H31NO	106010-22-4	53
3		Tetradecanamide	227	C14H29NO	000638-58-4	43
4		Decanamide-	171	C10H21NO	002319-29-1	38
5		Octadecanamide	283	C18H37NO	000124-26-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126308.D
Acq On : 21 Dec 2021 21:18
Operator : JU/CG
Sample : M5184-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3

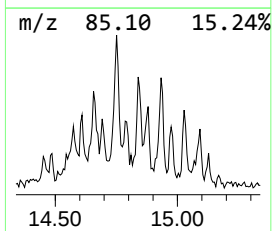
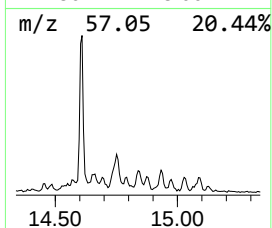
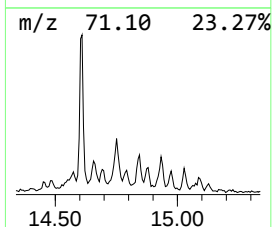
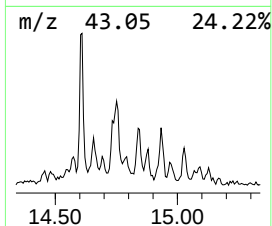
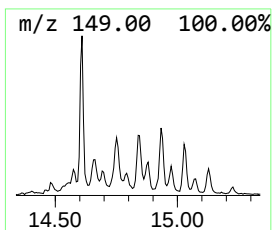
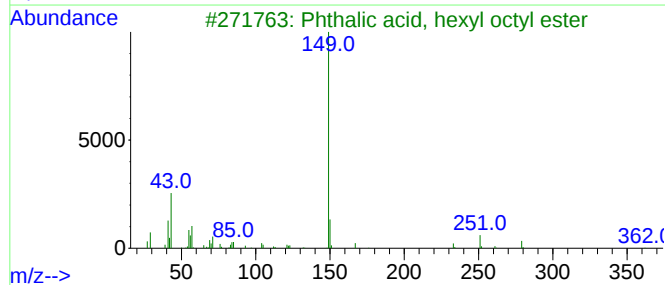
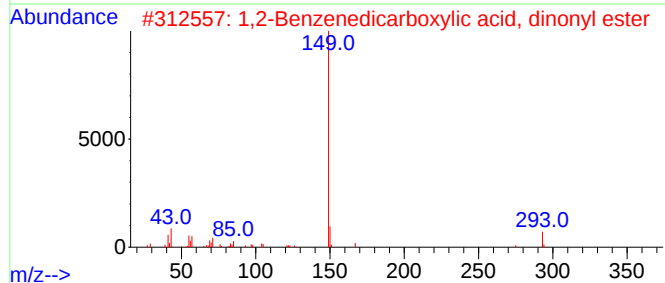
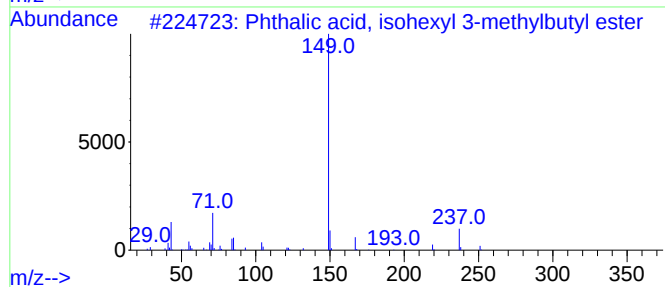
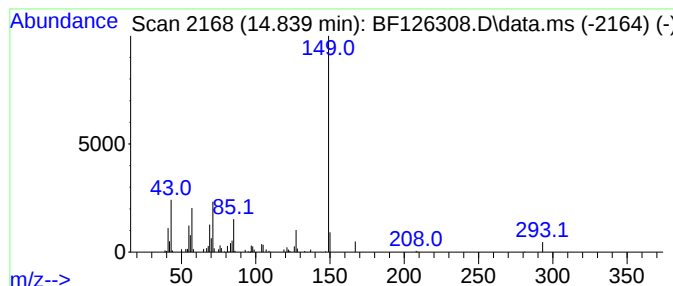
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phthalic acid, isohexyl 3-m... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	2.14 ng	116725	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, isohexyl 3-methyl...	320	C19H28O4	1000356-80-6	64
2			1,2-Benzenedicarboxylic acid, di...	418	C26H42O4	000084-76-4	59
3			Phthalic acid, hexyl octyl ester	362	C22H34O4	1000424-04-5	53
4			Phthalic acid, 3-methylbutyl pen...	306	C18H26O4	1000356-80-5	50
5			Phthalic acid, ethyl tetradecyl ...	390	C24H38O4	1000309-00-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126308.D
Acq On : 21 Dec 2021 21:18
Operator : JU/CG
Sample : M5184-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3

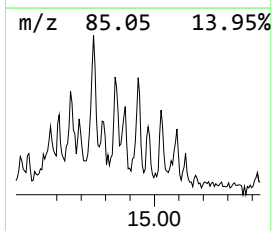
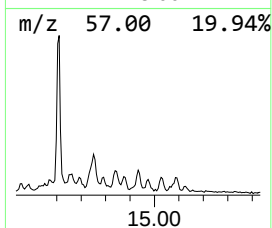
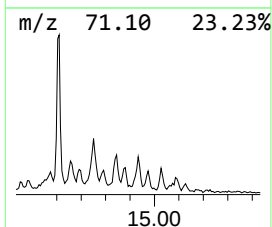
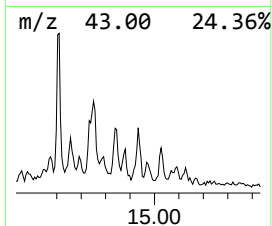
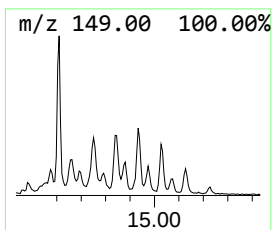
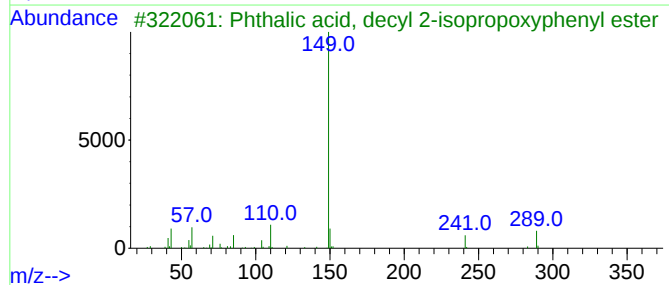
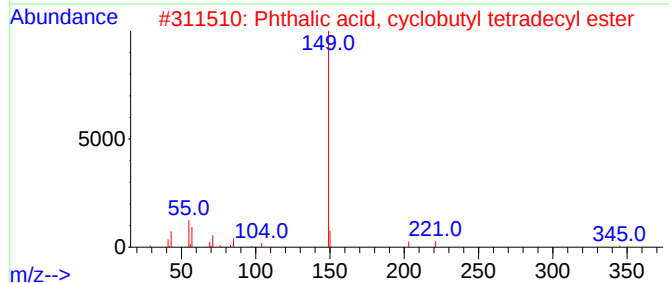
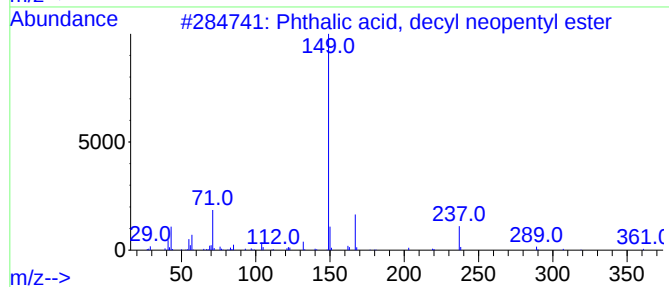
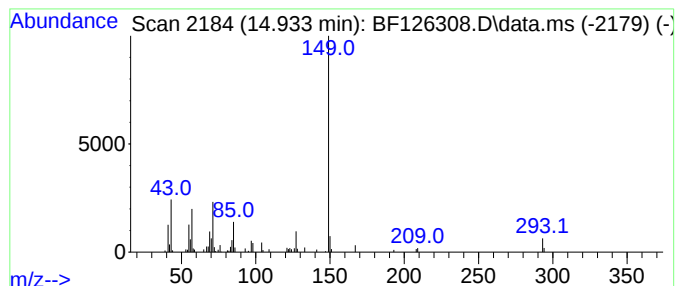
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phthalic acid, decyl neopen... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	2.11 ng	114929	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, decyl neopentyl e...	376	C23H36O4	1000315-30-3	59
2			Phthalic acid, cyclobutyl tetrad...	416	C26H40O4	1000314-90-9	59
3			Phthalic acid, decyl 2-isopropox...	440	C27H36O5	1000309-83-7	59
4			Phthalic acid, 3-fluorophenyl he...	498	C31H43FO4	1000356-66-2	59
5			Phthalic acid, decyl 3,5-dimethy...	410	C26H34O4	1000309-79-0	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126308.D
Acq On : 21 Dec 2021 21:18
Operator : JU/CG
Sample : M5184-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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
Butane, 2-metho...	2.116	6.5	ng	371376	1	6.816	1148700	20.0
2-Pyrrolidinone...	6.957	22.0	ng	1262470	1	6.816	1148700	20.0
7,9-Di-tert-but...	11.733	22.2	ng	1841060	4	11.339	1659040	20.0
9-Acetylphenant...	11.916	5.5	ng	459176	4	11.339	1659040	20.0
Triphenylphosph...	14.068	5.2	ng	382675	5	13.974	1476920	20.0
1,3-Benzenedica...	14.610	10.5	ng	775037	5	13.974	1476920	20.0
9-Octadecenamid...	14.739	3.3	ng	181759	6	15.421	1089930	20.0
Phthalic acid, ...	14.839	2.1	ng	116725	6	15.421	1089930	20.0
Phthalic acid, ...	14.933	2.1	ng	114929	6	15.421	1089930	20.0