

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
 Data File : BF131120.D
 Acq On : 10 Nov 2022 13:24
 Operator : CG\JU
 Sample : N5378-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-15-20221028-12.5-13.5

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-BF110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131120.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	10	16	24	rVB	312323	403449	24.23%	3.362%
2	2.293	30	35	40	rBV	32529	39363	2.36%	0.328%
3	5.110	510	514	522	rBV	188608	221497	13.30%	1.846%
4	5.510	577	582	585	rBV	1733165	1597794	95.95%	13.313%
5	6.516	748	753	756	rBV	1785239	1665280	100.00%	13.875%
6	6.887	812	816	820	rBV	614146	469631	28.20%	3.913%
7	7.451	907	912	915	rBV	1133116	987753	59.31%	8.230%
8	8.081	1015	1019	1030	rBV5	17559	44411	2.67%	0.370%
9	8.169	1030	1034	1038	rBV	516144	460042	27.63%	3.833%
10	9.251	1213	1218	1221	rBV	1605064	1447336	86.91%	12.059%
11	9.357	1233	1236	1248	rVB	43024	49876	3.00%	0.416%
12	9.934	1330	1334	1337	rBV	620418	518180	31.12%	4.317%
13	10.722	1464	1468	1472	rBV	1045746	896852	53.86%	7.473%
14	11.428	1584	1588	1591	rBV	552870	484305	29.08%	4.035%
15	11.492	1596	1599	1603	rVB2	18267	19543	1.17%	0.163%
16	11.810	1648	1653	1656	rVB3	22180	21324	1.28%	0.178%
17	12.039	1689	1692	1696	rBV4	14410	17541	1.05%	0.146%
18	12.110	1698	1704	1708	rBV3	17579	26278	1.58%	0.219%
19	12.204	1717	1720	1722	rBV	44508	44351	2.66%	0.370%
20	12.369	1742	1748	1752	rBV	76080	67223	4.04%	0.560%
21	12.445	1757	1761	1764	rBV	29094	34917	2.10%	0.291%
22	12.516	1770	1773	1776	rBV	65486	47906	2.88%	0.399%
23	12.604	1785	1788	1790	rVB2	23337	17396	1.04%	0.145%
24	12.639	1790	1794	1797	rBV	34291	31810	1.91%	0.265%
25	12.675	1797	1800	1804	rVB2	24329	25675	1.54%	0.214%
26	12.804	1819	1822	1829	rBV5	9465	17859	1.07%	0.149%
27	12.869	1829	1833	1837	rBV	43299	52035	3.12%	0.434%
28	13.016	1854	1858	1861	rVV	1572278	1388358	83.37%	11.568%
29	13.086	1865	1870	1876	rBV7	10788	19926	1.20%	0.166%
30	13.269	1898	1901	1905	rBV3	10926	19998	1.20%	0.167%
31	13.974	2015	2021	2029	rBV3	24431	62480	3.75%	0.521%
32	14.074	2034	2038	2041	rVV	407016	342071	20.54%	2.850%
33	14.098	2041	2042	2046	rVV	30574	17516	1.05%	0.146%
34	14.169	2046	2054	2058	rVB	58471	71018	4.26%	0.592%
35	15.127	2213	2217	2220	rBV	19011	26246	1.58%	0.219%
36	15.504	2278	2281	2285	rBV	18109	22463	1.35%	0.187%

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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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.568	2287	2292	2297	rBV	241932	322199	19.35%	2.685%
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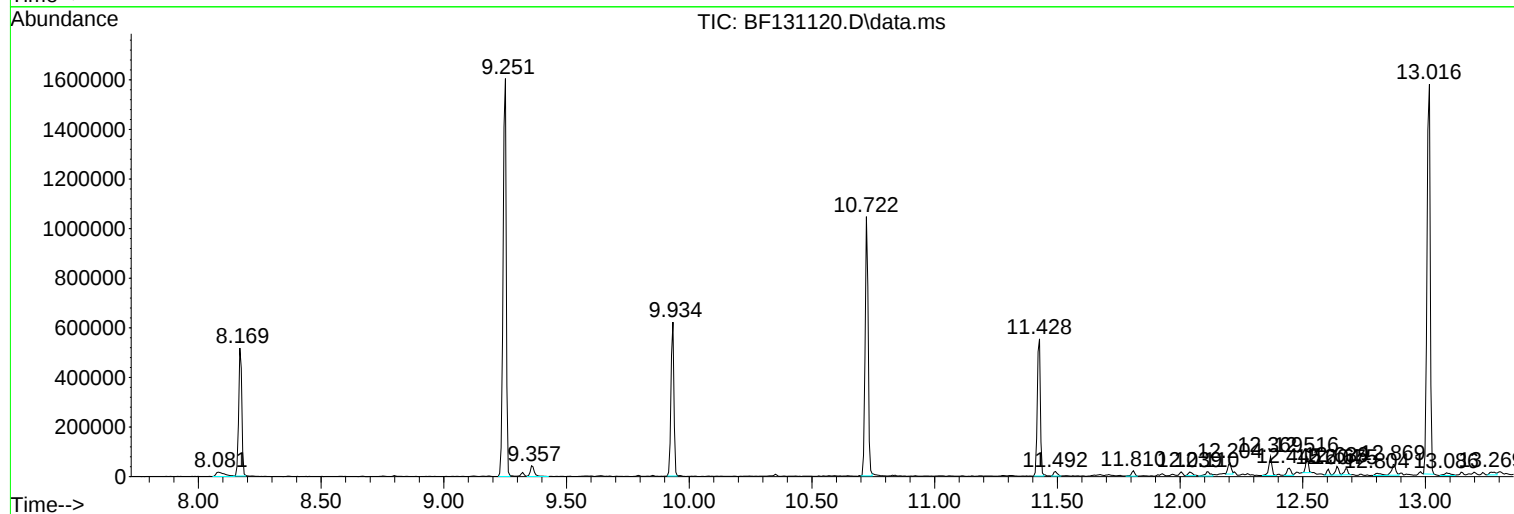
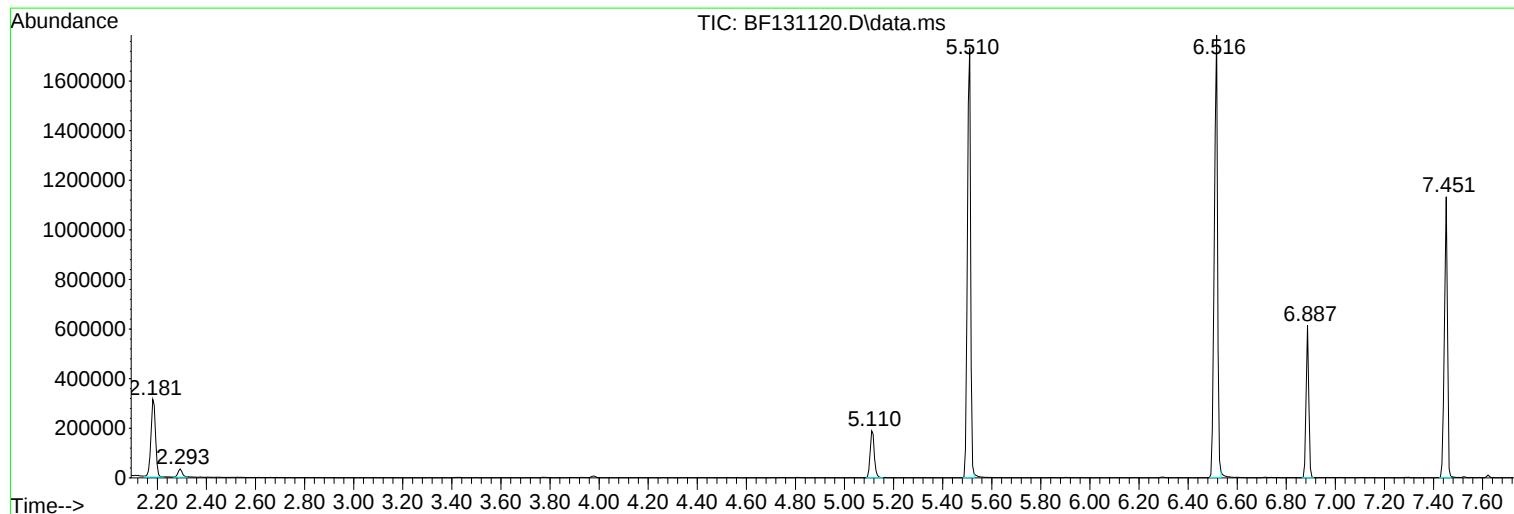
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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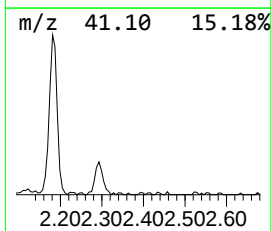
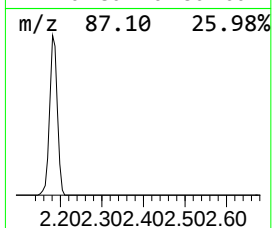
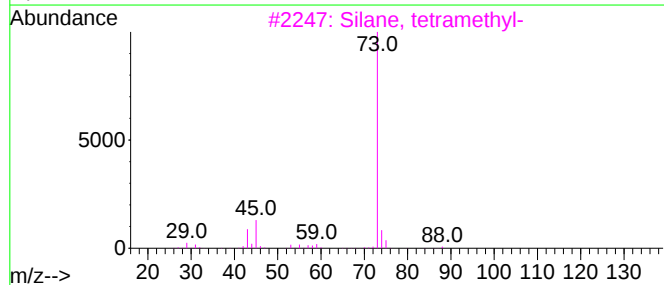
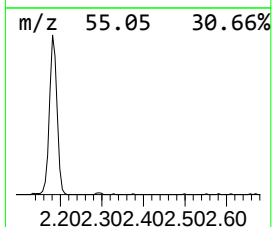
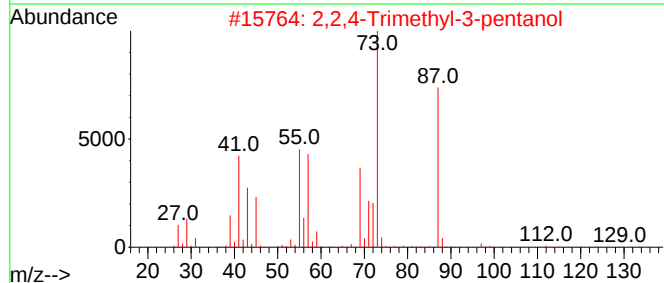
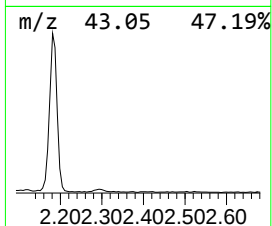
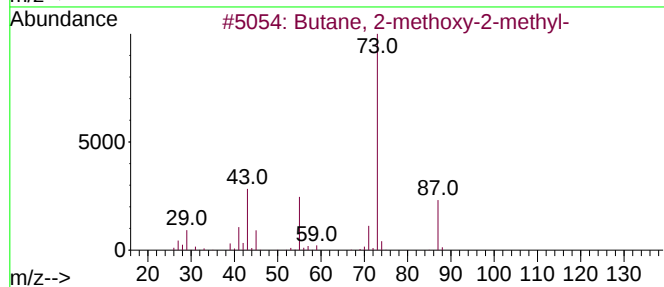
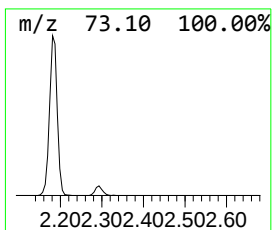
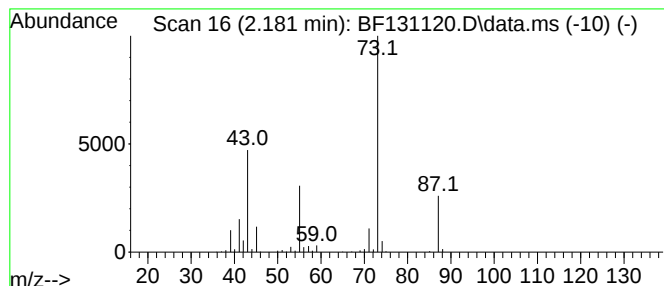
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	17.18 ng	403449	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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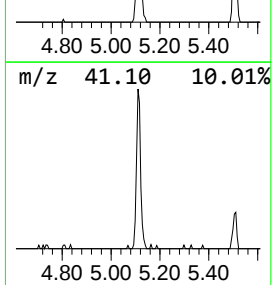
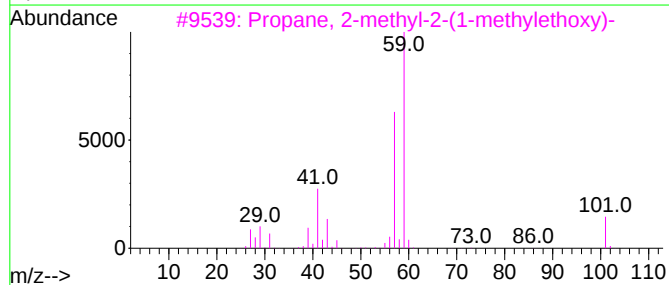
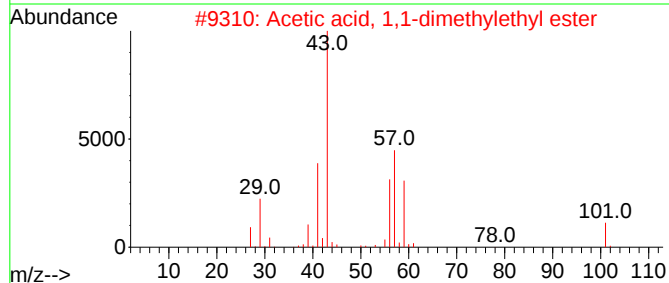
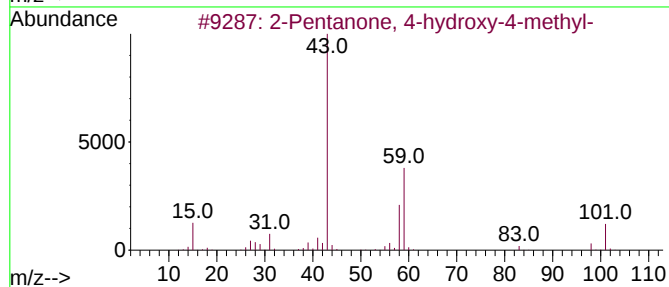
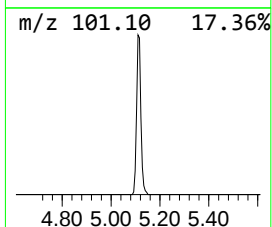
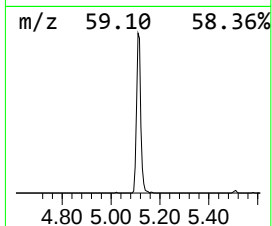
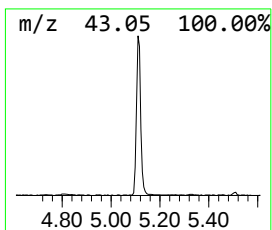
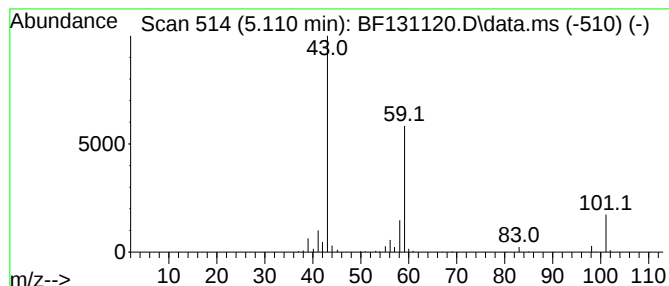
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	9.43 ng	221497	1,4-Dichlorobenzene-d4	6.887

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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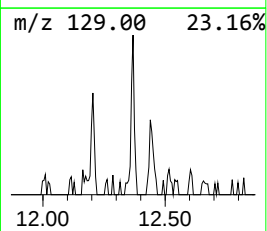
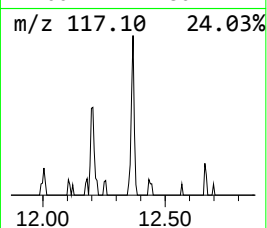
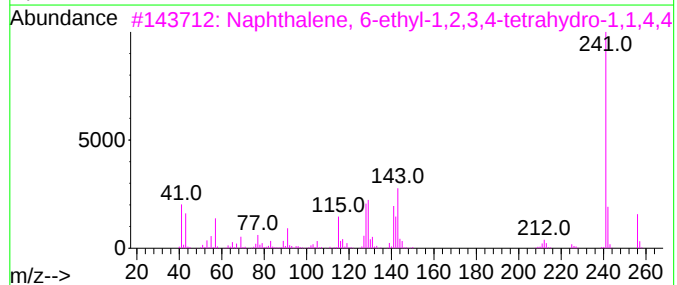
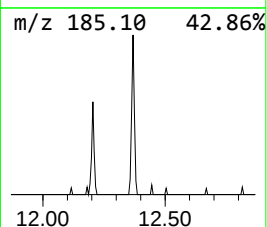
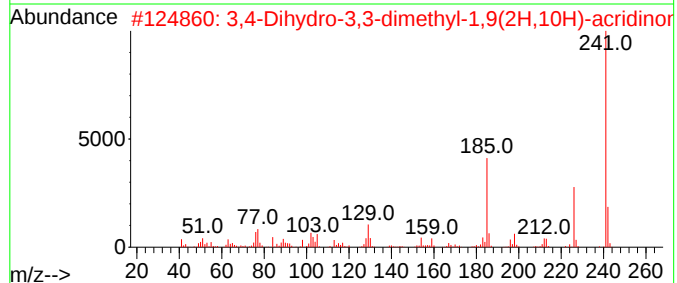
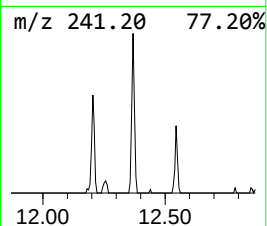
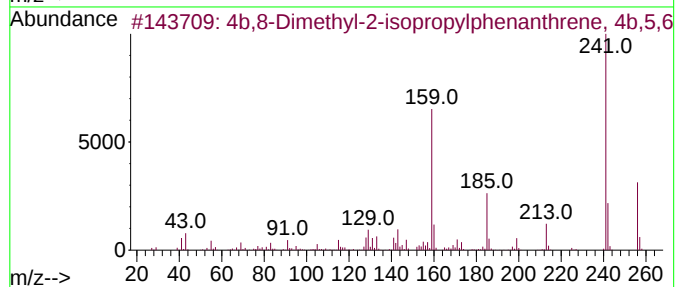
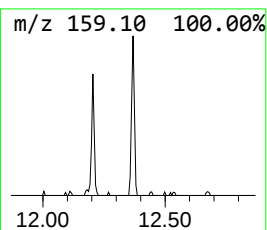
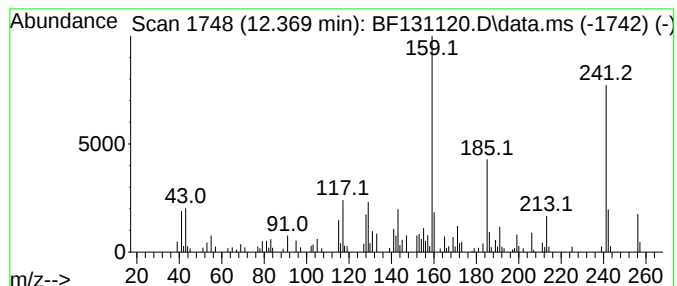
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4b,8-Dimethyl-2-isopropylph... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.369	2.78 ng	67223	Phenanthrene-d10	11.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4b,8-Dimethyl-2-isopropylphenant...	256	C19H28	1000197-14-1	98
2			3,4-Dihydro-3,3-dimethyl-1,9(2H,...	241	C15H15NO2	1010212-95-2	43
3			Naphthalene, 6-ethyl-1,2,3,4-tet...	256	C19H28	301643-35-6	42
4			s-Indacen-1(2H)-one, 3,5,6,7-tet...	256	C18H24O	038754-94-8	42
5			Benzene, 1,1'-(1-methylethyliden...	256	C17H20O2	001568-83-8	30



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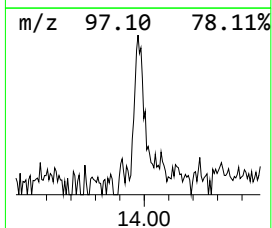
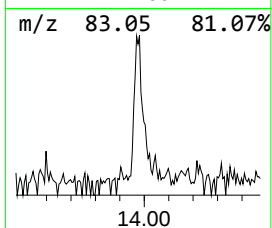
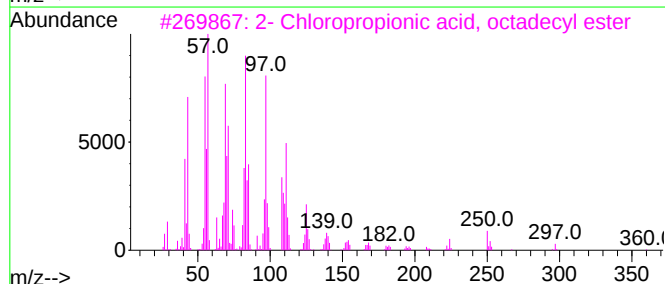
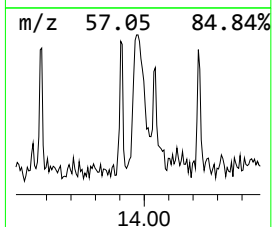
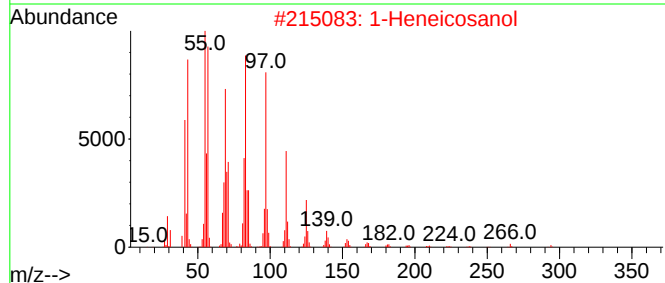
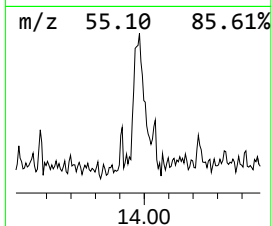
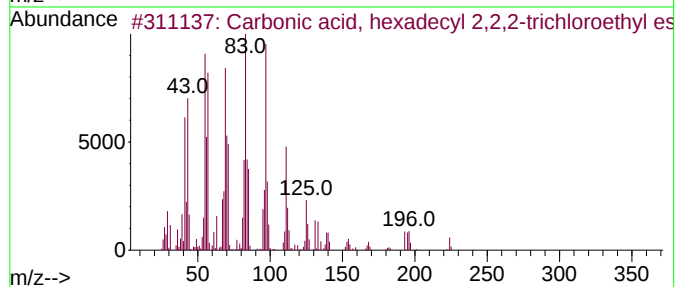
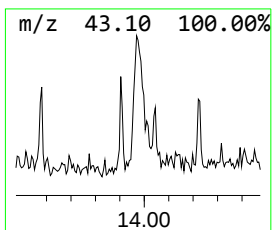
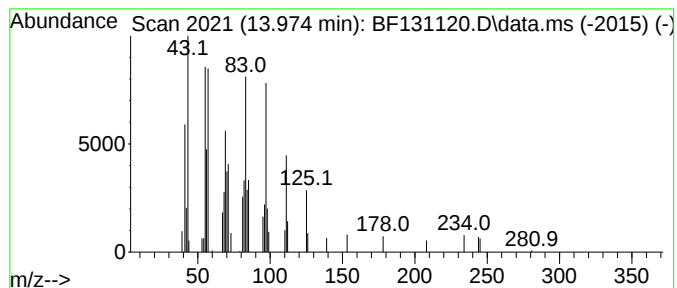
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Peak Number 4 Carbonic acid, hexadecyl 2,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	3.65 ng	62480	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	91
3			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4			1-Nonadecene	266	C19H38	018435-45-5	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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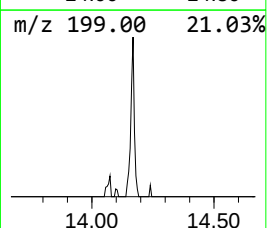
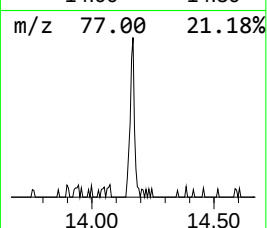
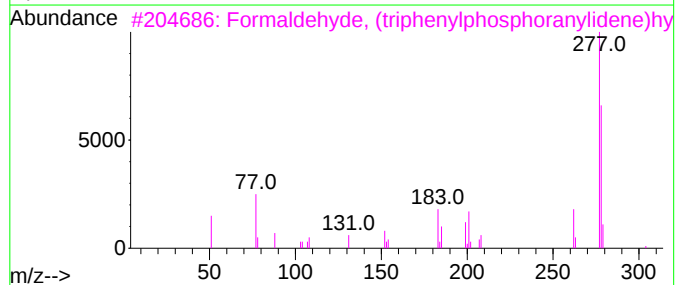
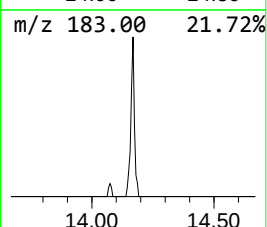
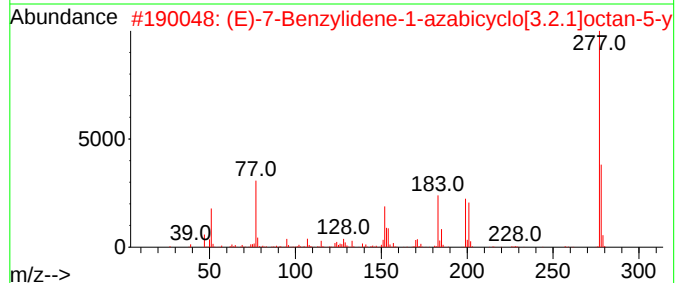
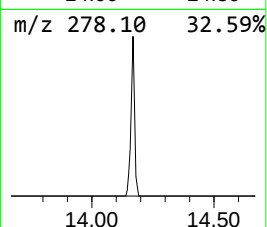
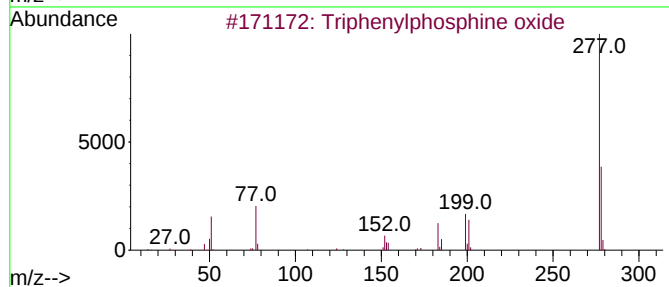
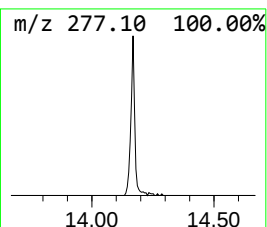
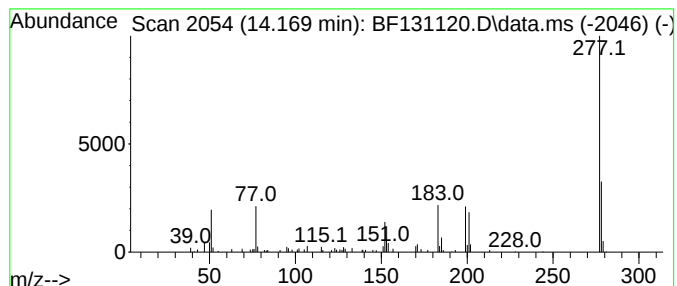
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	4.15 ng	71018	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	43
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
4			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	17
5			1,5-Dioxa-2,4,6,8-tetrasilacyclo...	292	C10H28O2Si4	015261-06-0	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131120.D
Acq On : 10 Nov 2022 13:24
Operator : CG\JU
Sample : N5378-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15-20221028-12.5-13.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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
Butane, 2-metho...	2.181	17.2	ng	403449	1	6.887	469631	20.0
2-Pentanone, 4-...	5.110	9.4	ng	221497	1	6.887	469631	20.0
4b,8-Dimethyl-2...	12.369	2.8	ng	67223	4	11.428	484305	20.0
Carbonic acid, ...	13.974	3.6	ng	62480	5	14.074	342071	20.0
Triphenylphosph...	14.169	4.2	ng	71018	5	14.074	342071	20.0