

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
 Data File : BF138373.D
 Acq On : 27 Jun 2024 18:39
 Operator : CG\JU
 Sample : P3076-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 7-N-1

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-BF061224.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138373.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	8	15	20	rBV	2078557	2568784	68.91%	8.728%
2	3.404	221	224	234	rBV	25182	54338	1.46%	0.185%
3	5.098	508	512	523	rVB	231028	261527	7.02%	0.889%
4	5.504	577	581	585	rBV	3103025	3074654	82.48%	10.446%
5	6.516	748	753	756	rBV	3441603	3065063	82.22%	10.414%
6	6.881	811	815	818	rBV	1640170	1273395	34.16%	4.326%
7	7.439	905	910	913	rBV	2407477	2045373	54.87%	6.949%
8	7.692	950	953	957	rVB	100332	75743	2.03%	0.257%
9	8.157	1029	1032	1036	rBV	1841952	1610373	43.20%	5.471%
10	8.469	1081	1085	1094	rBV	130574	126895	3.40%	0.431%
11	9.233	1211	1215	1218	rBV	4740809	3727861	100.00%	12.666%
12	9.910	1327	1330	1334	rBV	1842499	1564814	41.98%	5.317%
13	10.010	1342	1347	1352	rVB2	70018	92155	2.47%	0.313%
14	10.698	1460	1464	1477	rBV	2007147	1651345	44.30%	5.611%
15	10.804	1479	1482	1490	rVB	115312	125131	3.36%	0.425%
16	11.398	1579	1583	1585	rBV	1459997	1228135	32.94%	4.173%
17	11.422	1585	1587	1590	rVV	149829	126596	3.40%	0.430%
18	11.469	1590	1595	1598	rVB	44534	50201	1.35%	0.171%
19	11.921	1669	1672	1676	rBV2	100860	103989	2.79%	0.353%
20	12.610	1785	1789	1792	rBV	333096	287058	7.70%	0.975%
21	12.833	1822	1827	1833	rBV	288891	320473	8.60%	1.089%
22	12.980	1848	1852	1855	rBV	3506784	2880076	77.26%	9.785%
23	13.874	2001	2004	2013	rBV	161770	208064	5.58%	0.707%
24	14.033	2026	2031	2034	rBV	1476235	1441794	38.68%	4.899%
25	14.057	2034	2035	2041	rVB	175999	127421	3.42%	0.433%
26	15.074	2204	2208	2211	rBV	125413	192473	5.16%	0.654%
27	15.374	2257	2259	2265	rVB	71662	86171	2.31%	0.293%
28	15.439	2267	2270	2276	rVB	94046	115125	3.09%	0.391%
29	15.504	2276	2281	2285	rBV	783404	947746	25.42%	3.220%

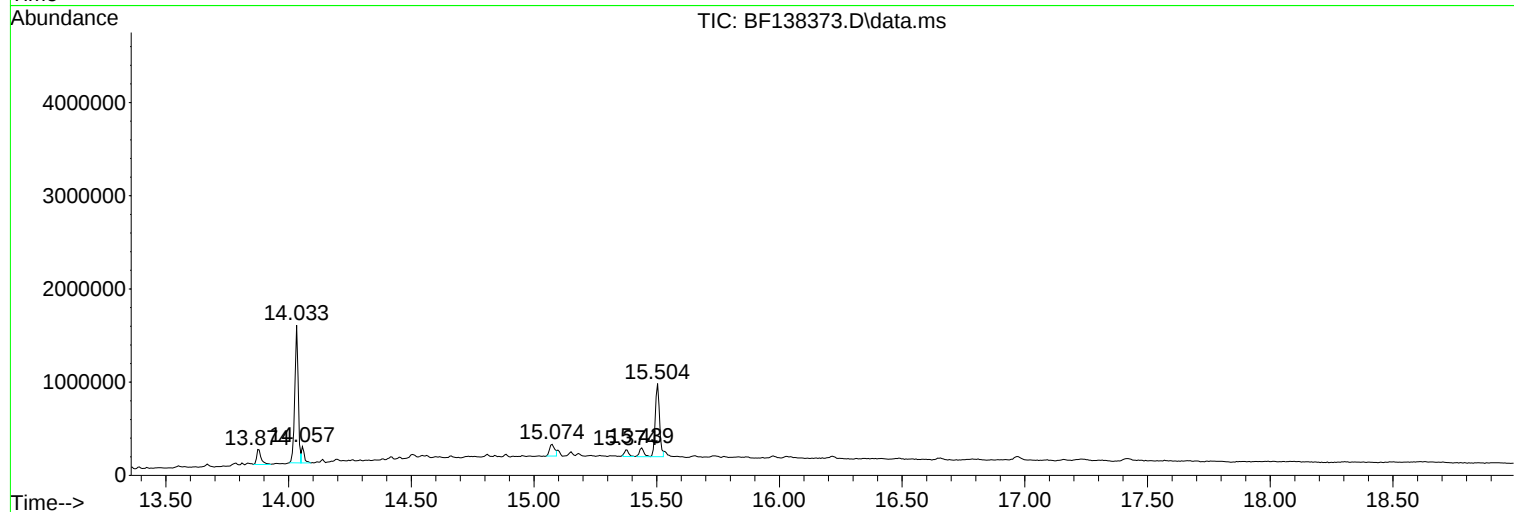
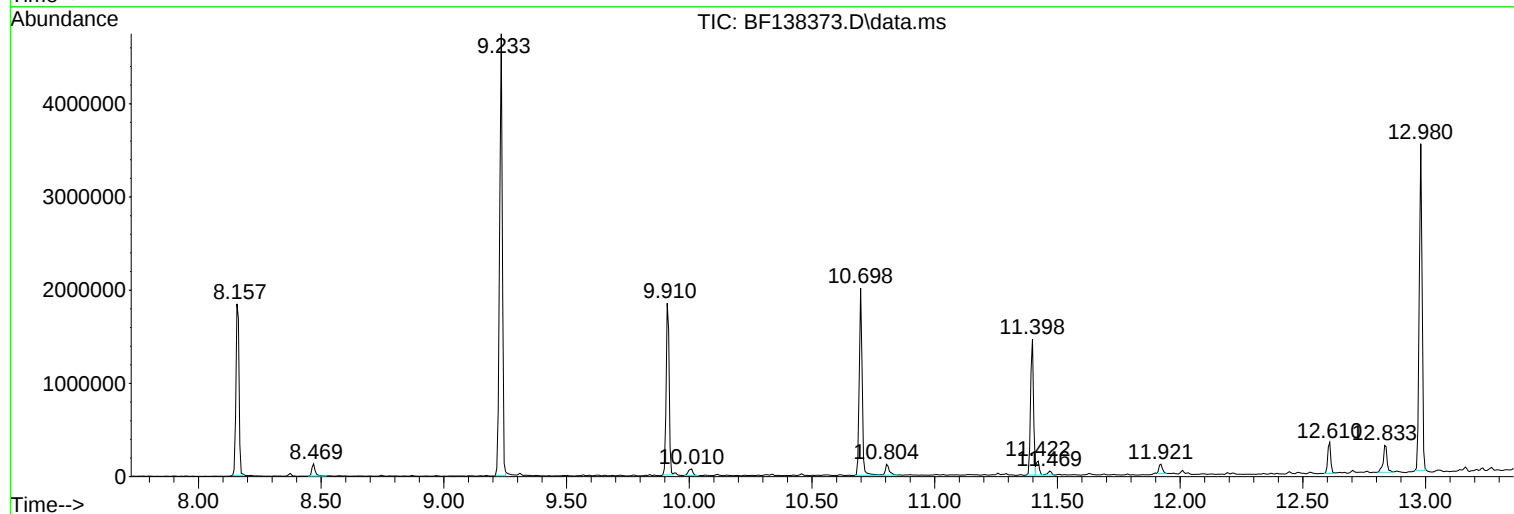
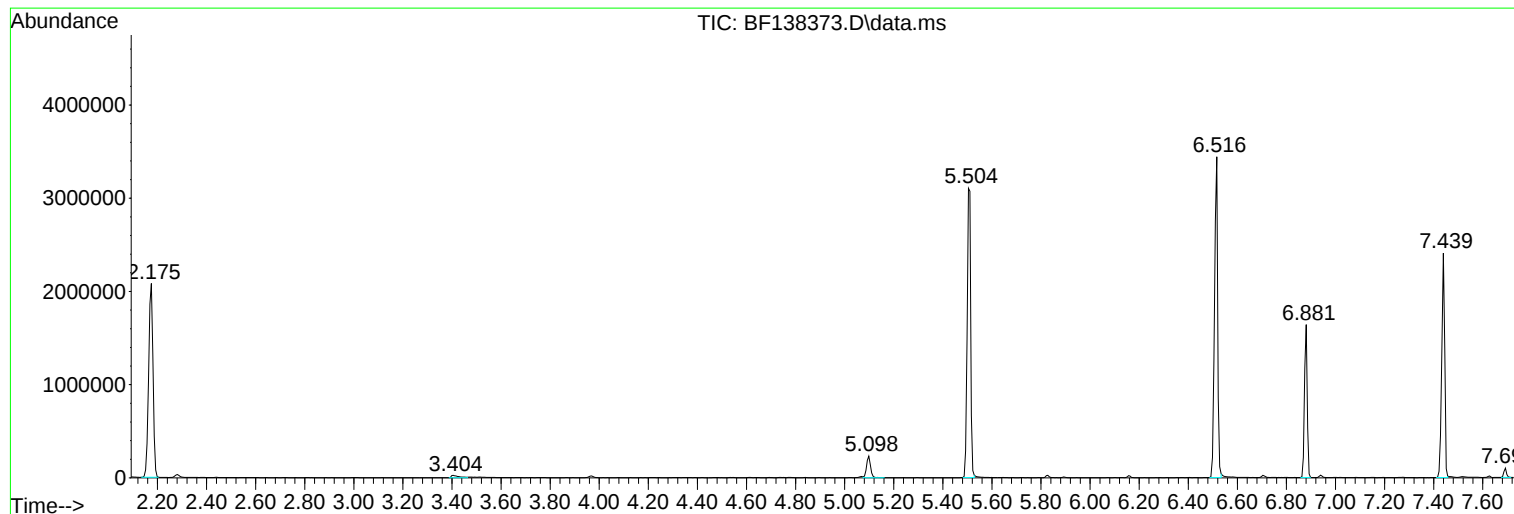
Sum of corrected areas: 29432773

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138373.D
Acq On : 27 Jun 2024 18:39
Operator : CG\JU
Sample : P3076-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-N-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138373.D
Acq On : 27 Jun 2024 18:39
Operator : CG\JU
Sample : P3076-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-N-1

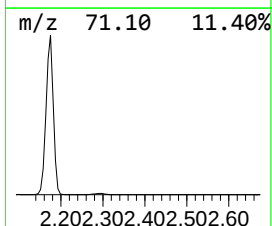
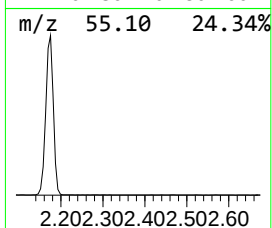
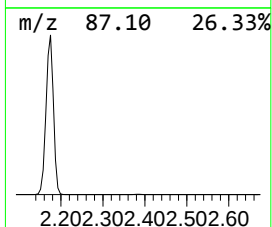
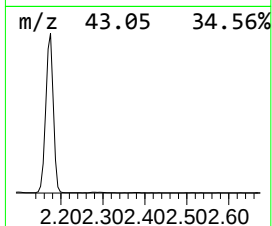
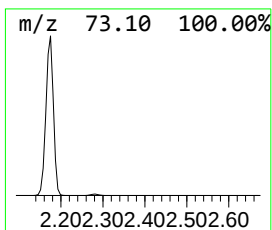
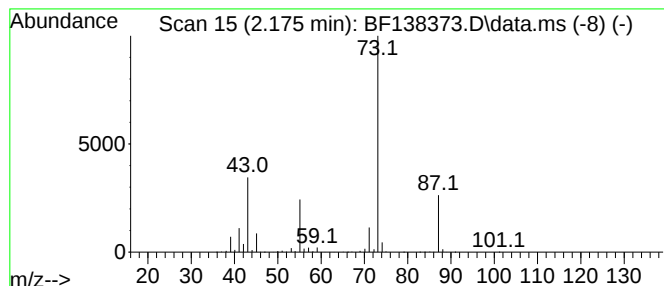
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.175	40.35 ng	2568780	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138373.D
Acq On : 27 Jun 2024 18:39
Operator : CG\JU
Sample : P3076-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-N-1

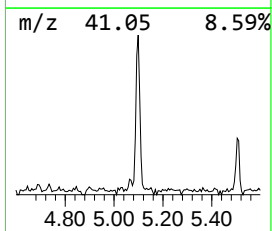
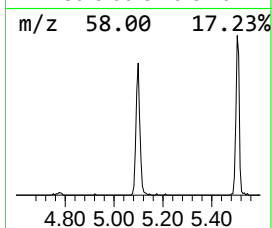
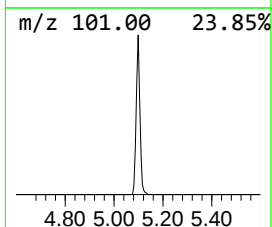
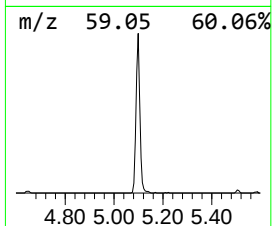
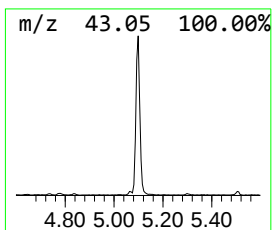
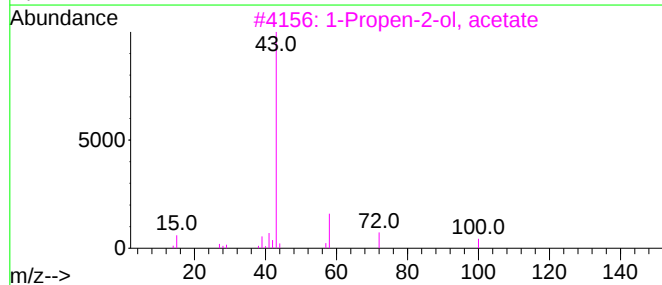
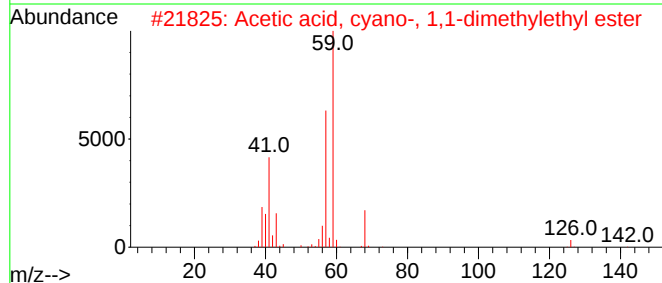
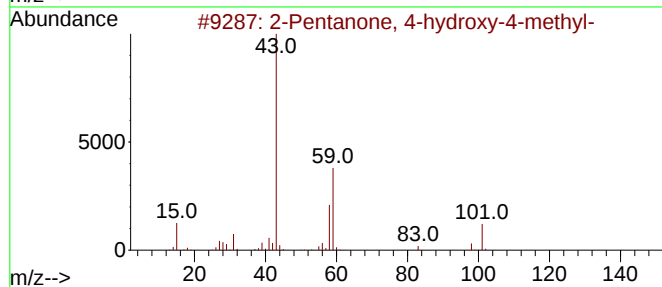
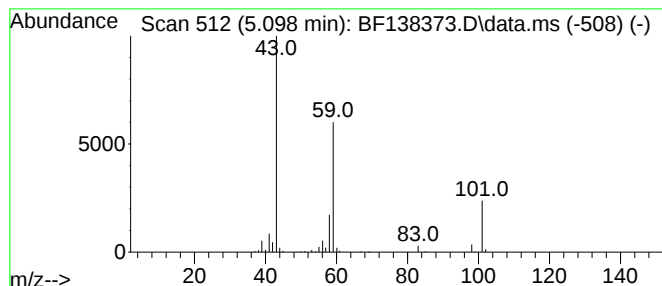
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.098	4.11 ng	261527	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138373.D
Acq On : 27 Jun 2024 18:39
Operator : CG\JU
Sample : P3076-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-N-1

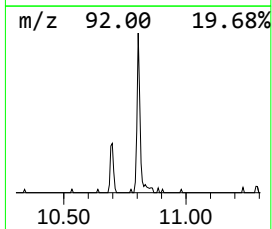
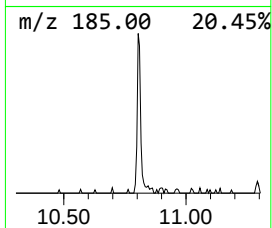
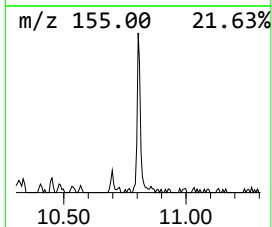
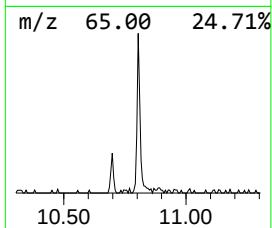
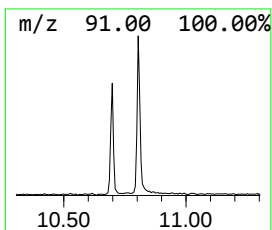
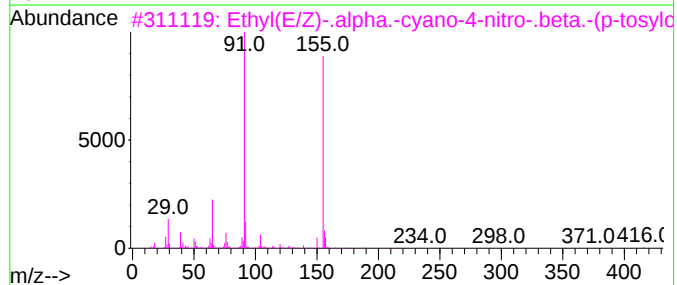
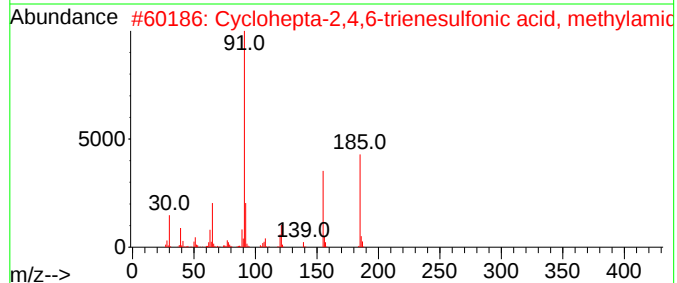
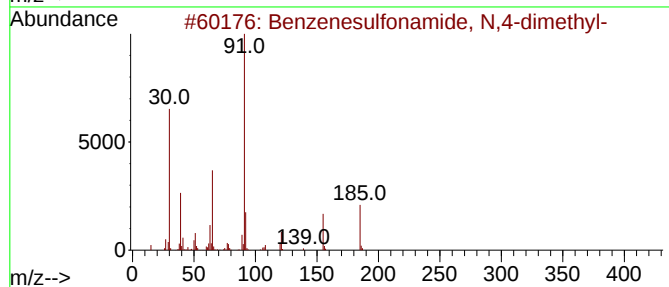
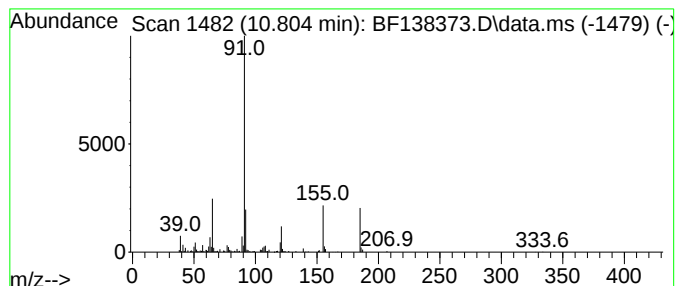
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	2.04 ng	125131	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2			Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	53
3			Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	47
4			Toluene-4-sulfonic acid, 2-benzy...	366	C18H22O6S	118653-93-3	47
5			Benzeneacetaldehyde	120	C8H8O	000122-78-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138373.D
Acq On : 27 Jun 2024 18:39
Operator : CG\JU
Sample : P3076-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-N-1

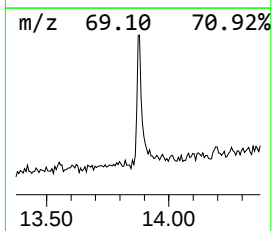
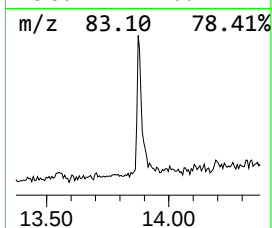
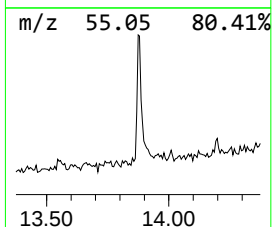
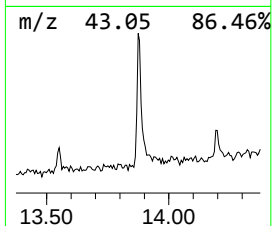
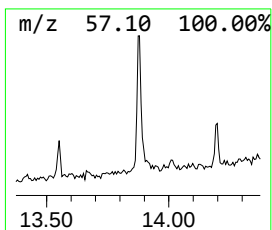
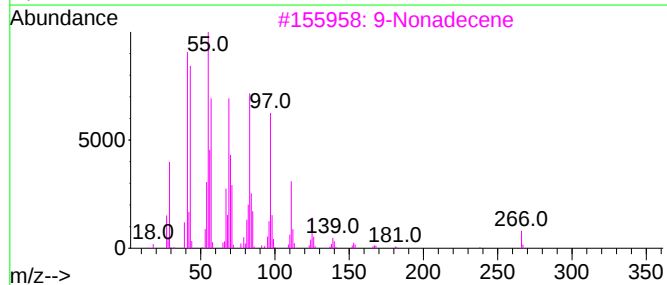
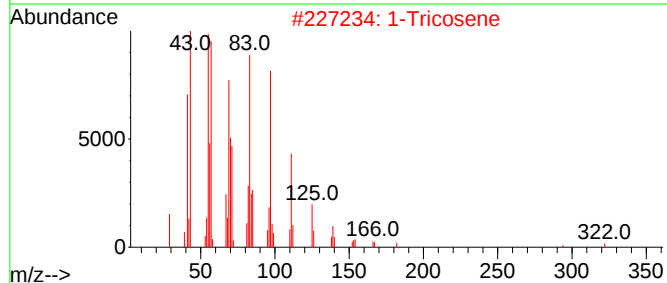
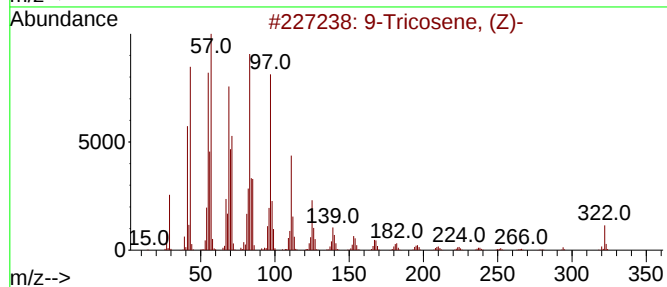
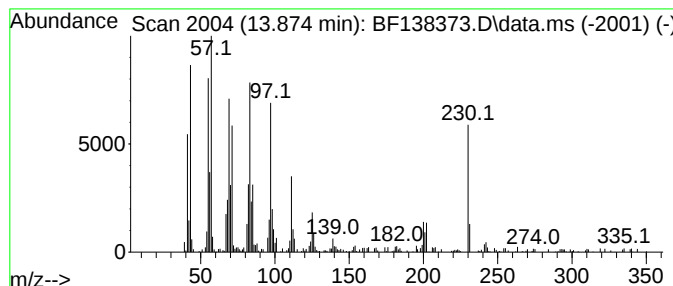
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Tricosene, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.89 ng	208064	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-			322	C23H46	027519-02-4	99
2	1-Tricosene			322	C23H46	018835-32-0	96
3	9-Nonadecene			266	C19H38	031035-07-1	91
4	Pentafluoropropionic acid, octad...			416	C21H37F5O2	959261-25-7	90
5	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138373.D
Acq On : 27 Jun 2024 18:39
Operator : CG\JU
Sample : P3076-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-N-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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...	2.175	40.4	ng	2568780	1	6.881	1273400	20.0
2-Pentanone, 4-...	5.098	4.1	ng	261527	1	6.881	1273400	20.0
Benzenesulfonam...	10.804	2.0	ng	125131	4	11.398	1228140	20.0
9-Tricosene, (Z)-	13.874	2.9	ng	208064	5	14.033	1441790	20.0