

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122723\
 Data File : BF136774.D
 Acq On : 27 Dec 2023 23:33
 Operator : CG\JU
 Sample : 06018-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136774.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	496	500	508	rVB	69726	90599	4.90%	0.735%
2	5.428	564	568	584	rBV	1587387	1429451	77.24%	11.597%
3	6.428	734	738	741	rBV	1427653	1444654	78.06%	11.721%
4	6.781	795	798	802	rBV	565601	441649	23.86%	3.583%
5	7.345	889	894	897	rBV	1100335	957495	51.74%	7.768%
6	8.057	1011	1015	1019	rBV	691687	579024	31.29%	4.698%
7	9.139	1194	1199	1202	rBV	2243350	1850725	100.00%	15.015%
8	9.816	1310	1314	1318	rBV	791959	618210	33.40%	5.016%
9	10.610	1445	1449	1458	rBV	835122	737950	39.87%	5.987%
10	11.310	1564	1568	1571	rBV	601550	550115	29.72%	4.463%
11	11.839	1655	1658	1662	rBV2	44967	51048	2.76%	0.414%
12	12.527	1771	1775	1779	rBV	30179	31633	1.71%	0.257%
13	12.757	1811	1814	1816	rVB	26322	24104	1.30%	0.196%
14	12.904	1834	1839	1842	rBV	1566936	1356513	73.30%	11.005%
15	13.839	1995	1998	2003	rVB6	47866	76624	4.14%	0.622%
16	13.963	2015	2019	2022	rBV	443983	385088	20.81%	3.124%
17	15.445	2266	2271	2274	rBV	296055	406041	21.94%	3.294%
18	16.186	2389	2397	2412	rVB4	304800	1294857	69.96%	10.505%

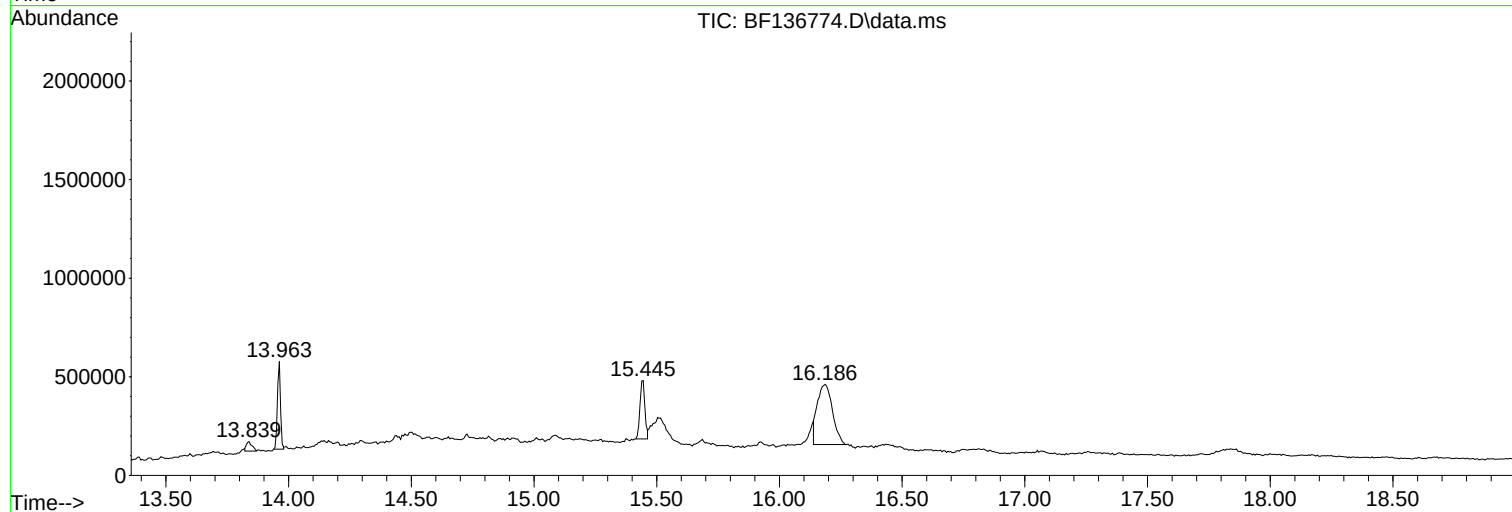
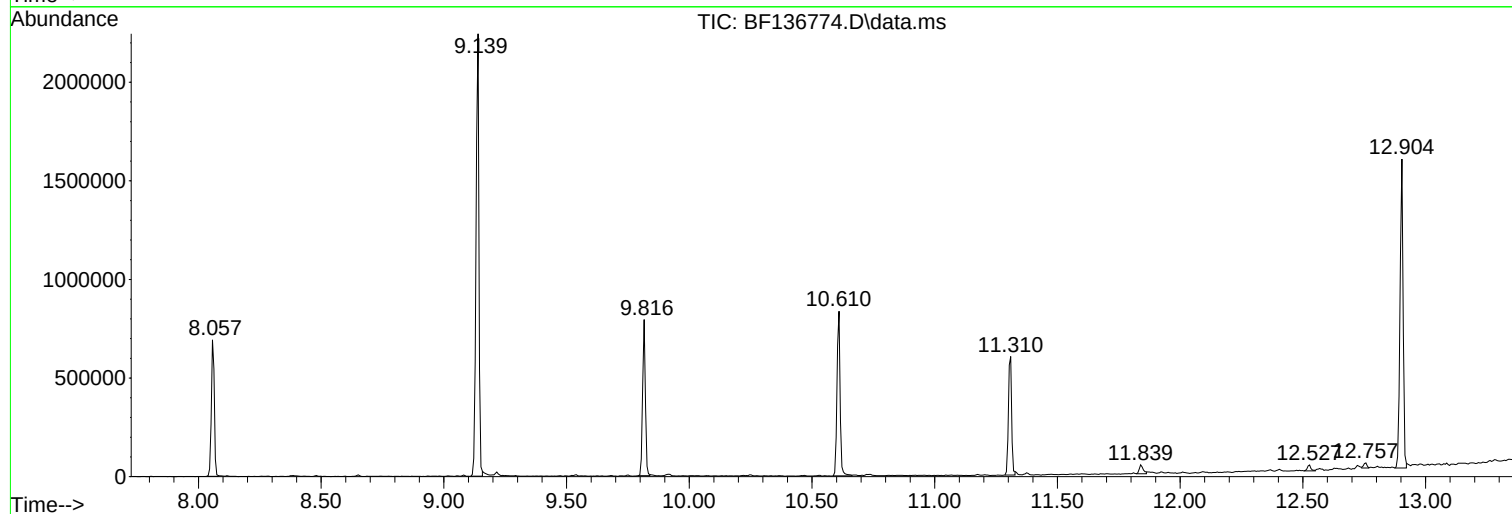
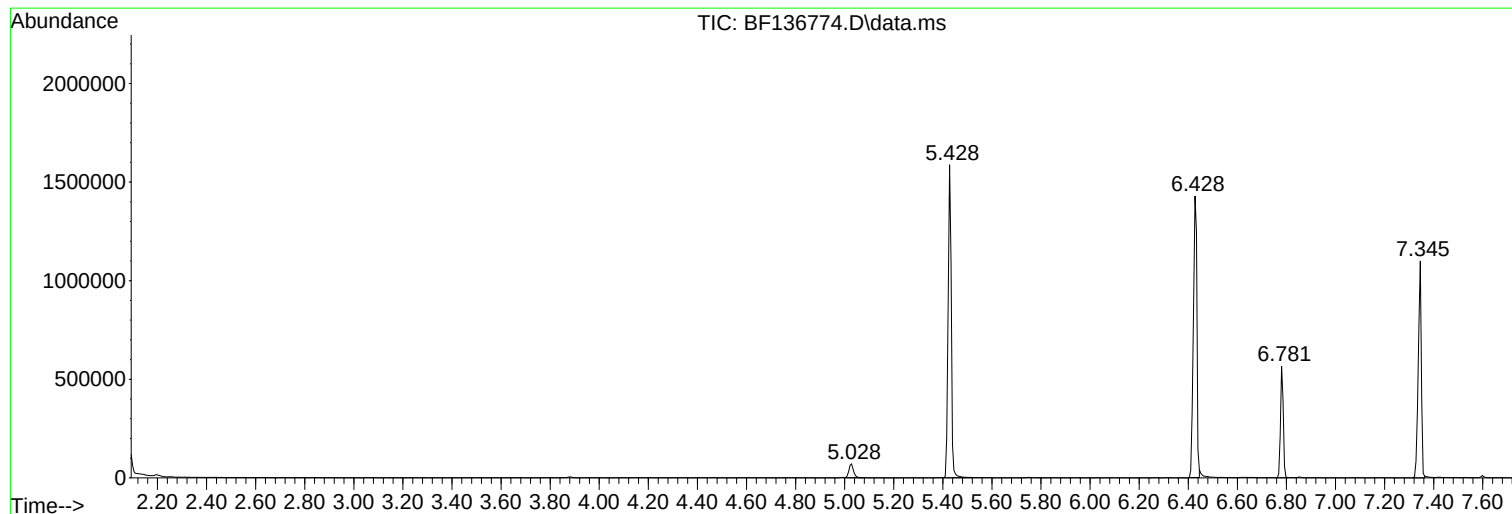
Sum of corrected areas: 12325780

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122723\
Data File : BF136774.D
Acq On : 27 Dec 2023 23:33
Operator : CG\JU
Sample : 06018-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF122723\
Data File : BF136774.D
Acq On : 27 Dec 2023 23:33
Operator : CG\JU
Sample : 06018-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

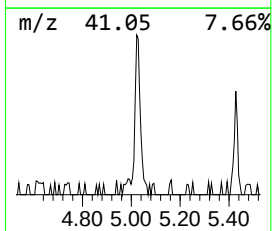
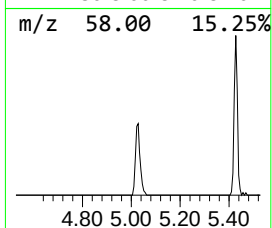
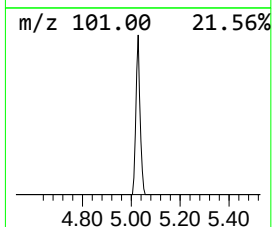
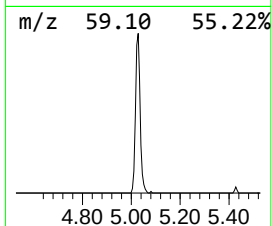
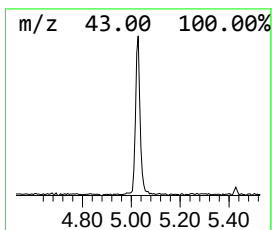
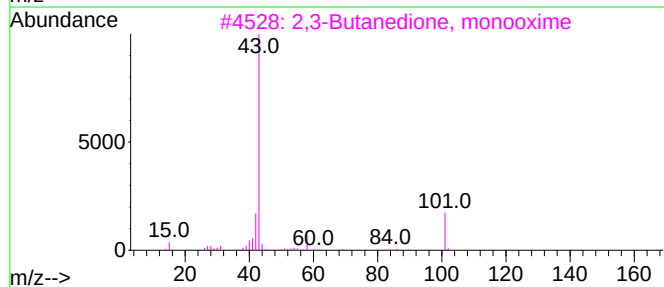
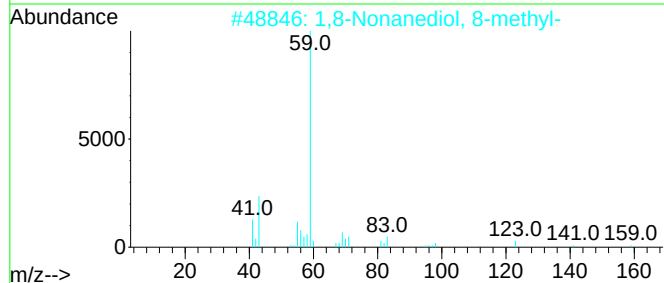
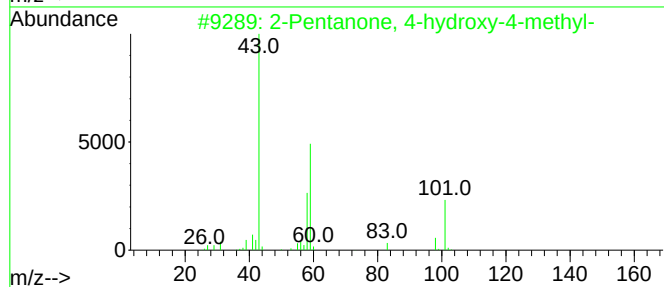
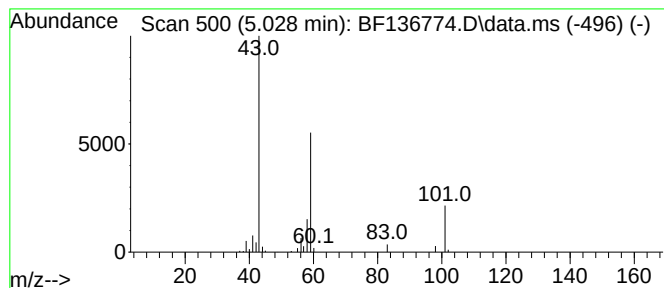
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	4.10 ng	90599	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122723\
Data File : BF136774.D
Acq On : 27 Dec 2023 23:33
Operator : CG\JU
Sample : 06018-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

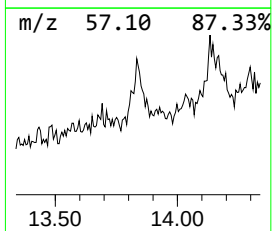
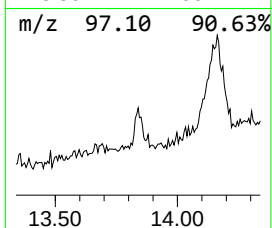
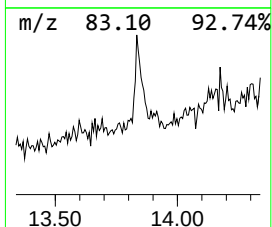
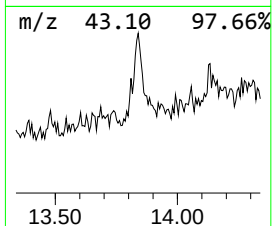
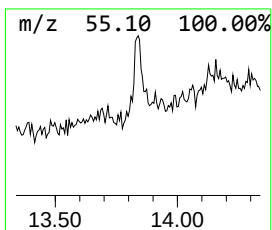
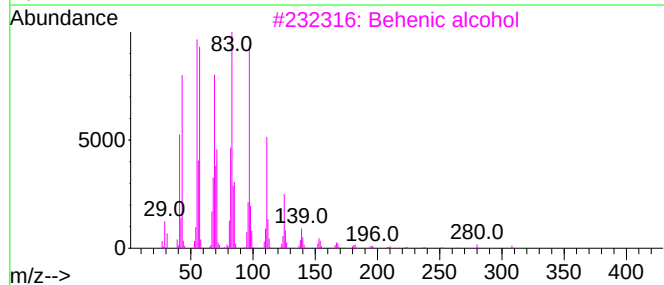
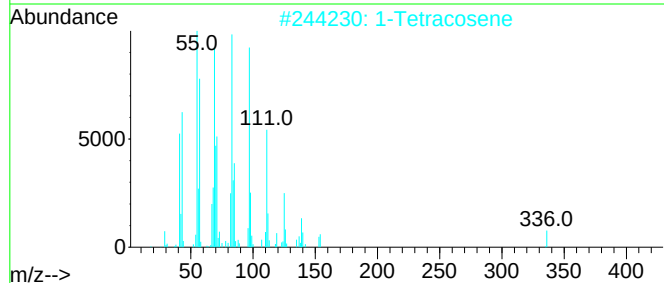
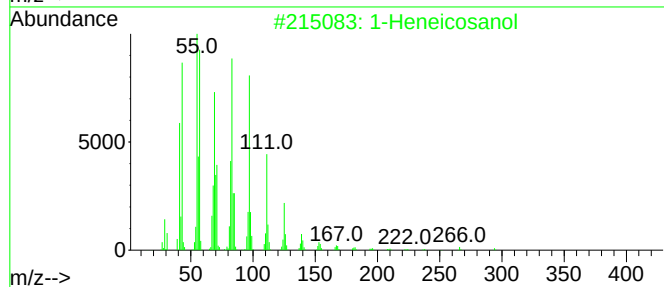
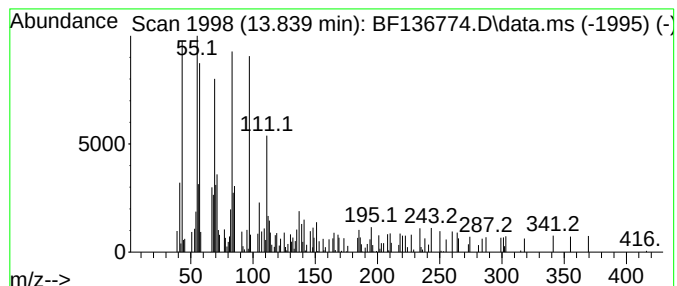
Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.839	3.98 ng	76624	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	87
2	1-Tetracosene	336	C24H48	010192-32-2	83
3	Behenic alcohol	326	C22H46O	000661-19-8	80
4	1-Hexacosene	364	C26H52	018835-33-1	80
5	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122723\
Data File : BF136774.D
Acq On : 27 Dec 2023 23:33
Operator : CG\JU
Sample : 06018-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

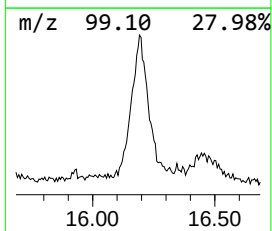
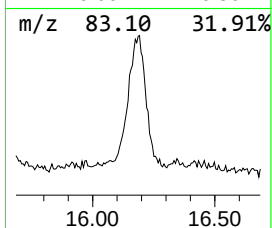
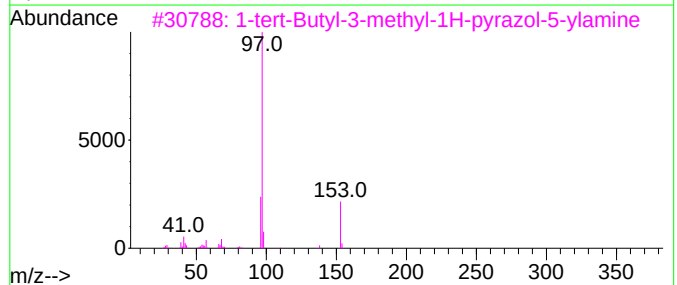
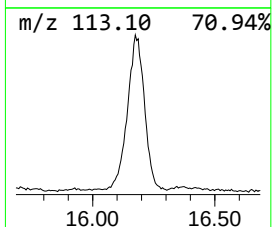
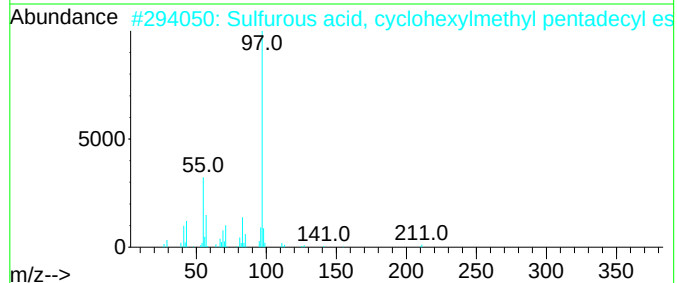
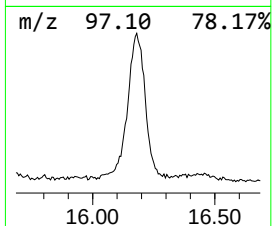
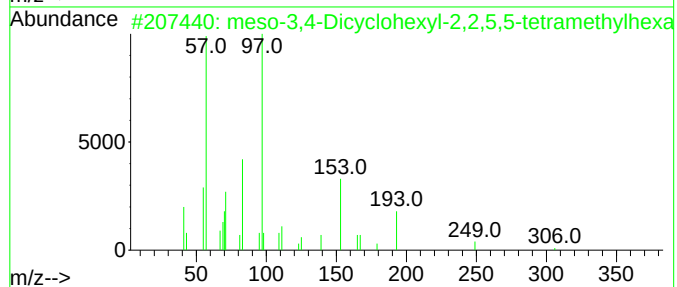
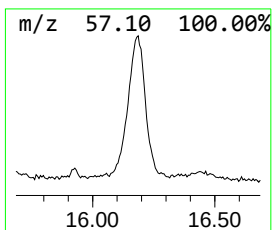
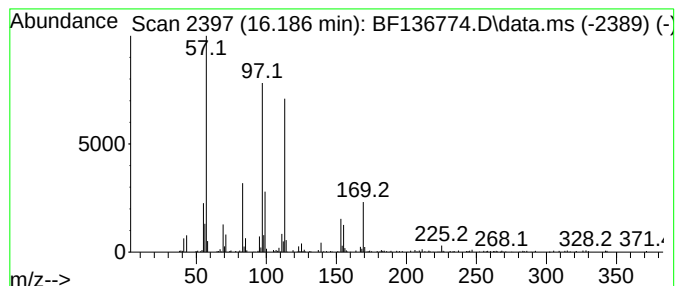
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown16.186 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.186	63.78 ng	1294860	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			meso-3,4-Dicyclohexyl-2,2,5,5-te...	306	C22H42	065149-86-2	46
2			Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	35
3			1-tert-Butyl-3-methyl-1H-pyrazol...	153	C8H15N3	141459-53-2	27
4			Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	22
5			1,2,4-Oxadiazol-5-amine, 3-(4-am...	264	C9H8N6O2S	1000351-26-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122723\
Data File : BF136774.D
Acq On : 27 Dec 2023 23:33
Operator : CG\JU
Sample : 06018-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
2-Pentanone, 4-...	5.028	4.1	ng	90599	1	6.781	441649	20.0
1-Heneicosanol	13.839	4.0	ng	76624	5	13.963	385088	20.0
unknown16.186	16.186	63.8	ng	1294860	6	15.445	406041	20.0