

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120722\
 Data File : BG055916.D
 Acq On : 7 Dec 2022 16:12
 Operator : CG/JU
 Sample : PB149462BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB149462BL

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_G\Methods\8270-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055916.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.196	319	325	340	rVB	104816	158848	6.61%	1.742%
2	5.690	402	409	420	rBV	455972	712789	29.65%	7.816%
3	7.317	678	686	701	rBV	457900	778105	32.37%	8.532%
4	8.158	823	829	838	rBV	77966	127862	5.32%	1.402%
5	9.333	1022	1029	1042	rVB	266616	470213	19.56%	5.156%
6	10.990	1303	1311	1322	rBV	111249	199500	8.30%	2.188%
7	13.416	1717	1724	1734	rBV	783021	1186002	49.33%	13.005%
8	14.797	1952	1959	1967	rBV	206290	319815	13.30%	3.507%
9	16.283	2205	2212	2234	rBV	621670	990037	41.18%	10.856%
10	17.535	2419	2425	2432	rBV	295121	447871	18.63%	4.911%
11	20.126	2860	2866	2871	rBV	1898734	2404129	100.00%	26.363%
12	21.818	3148	3154	3164	rVB	330664	553844	23.04%	6.073%
13	23.299	3403	3406	3414	rVB4	16092	30689	1.28%	0.337%
14	24.133	3543	3548	3554	rVB2	22131	45445	1.89%	0.498%
15	25.167	3710	3724	3737	rVB2	186689	625546	26.02%	6.860%
16	26.289	3909	3915	3922	rVB4	25237	68625	2.85%	0.753%

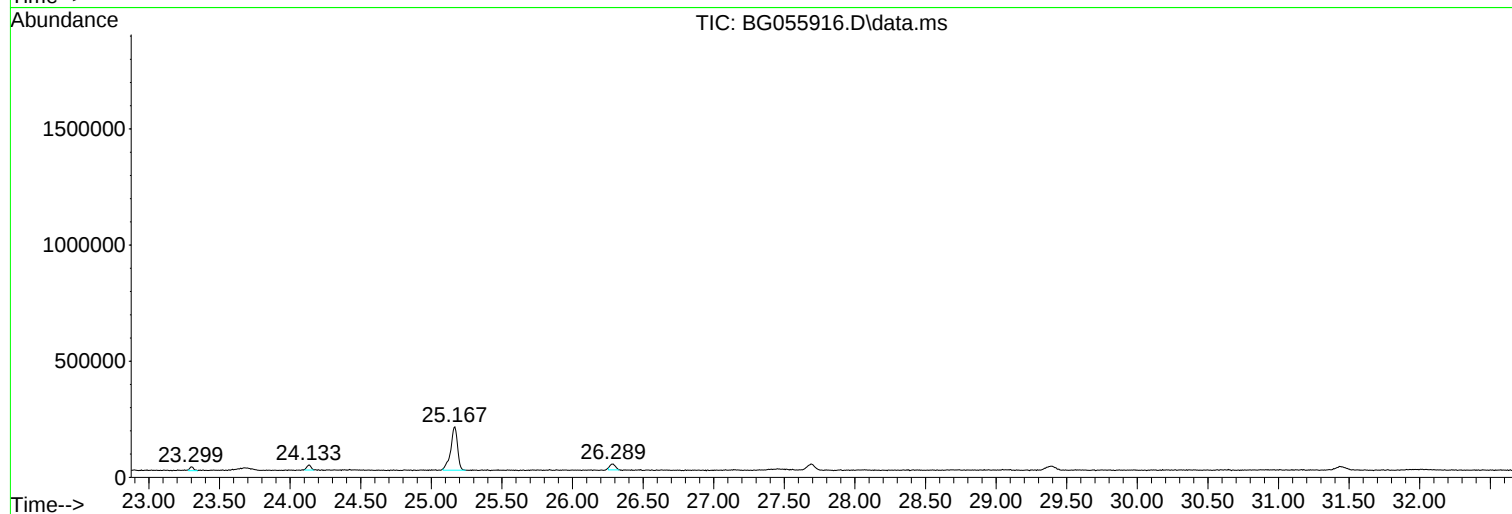
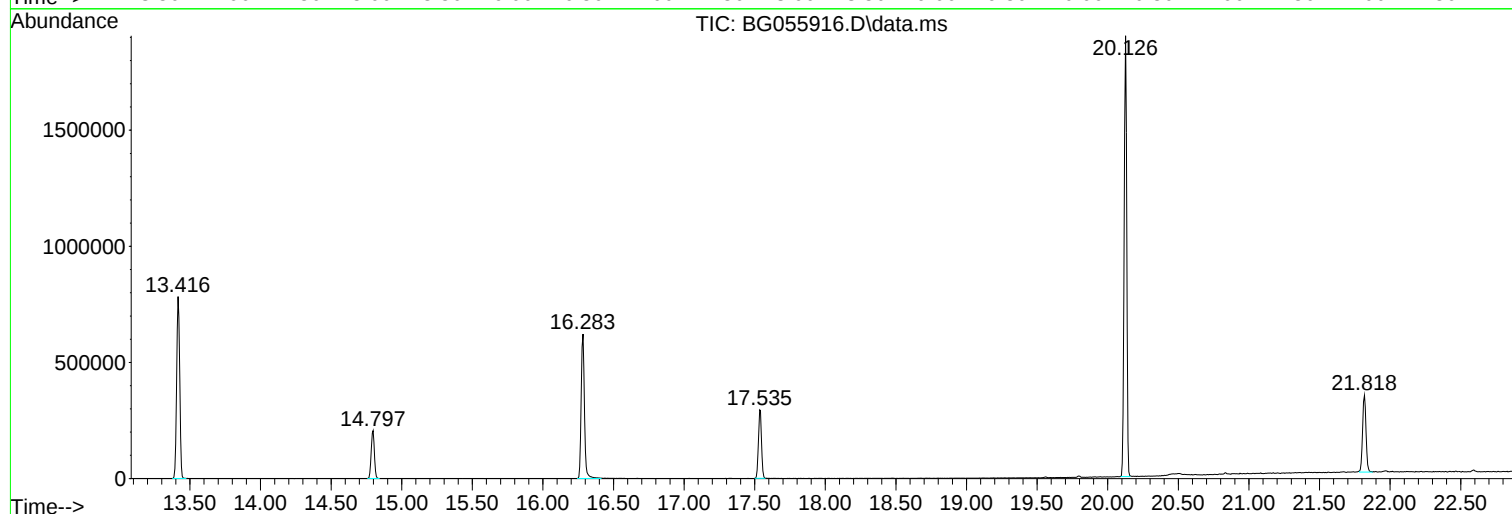
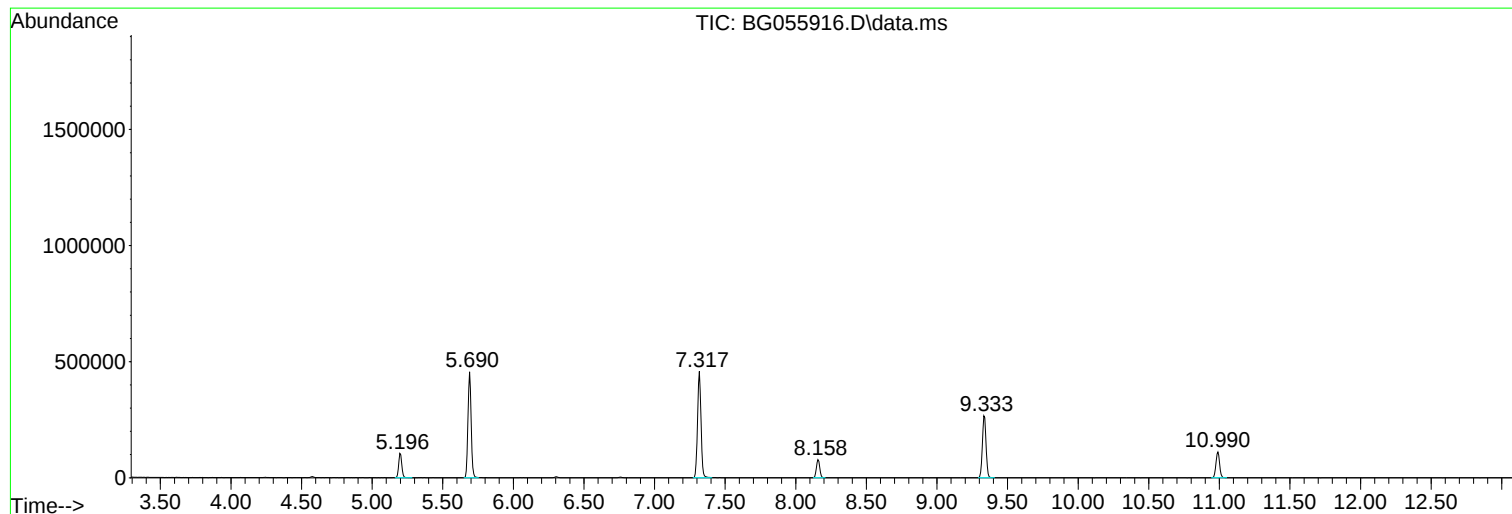
Sum of corrected areas: 9119320

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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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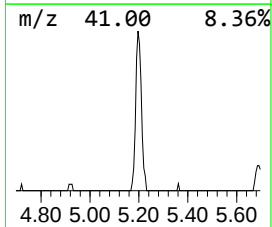
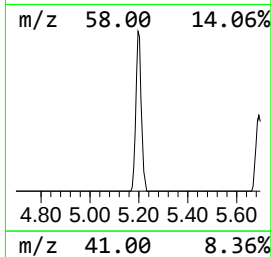
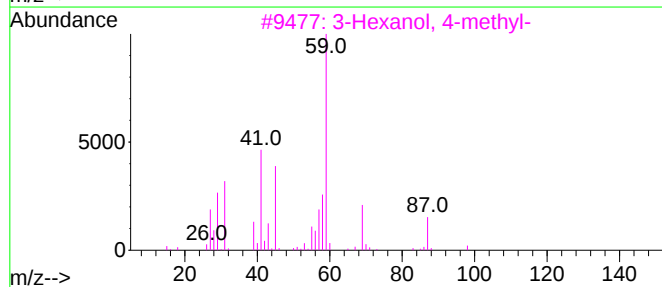
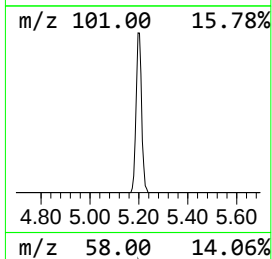
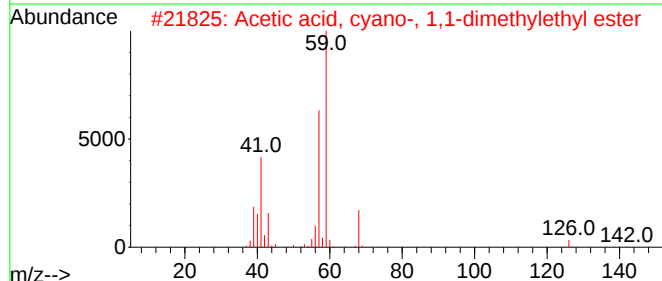
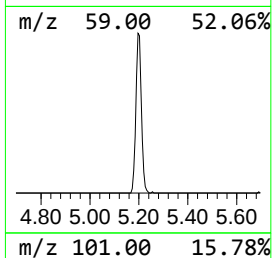
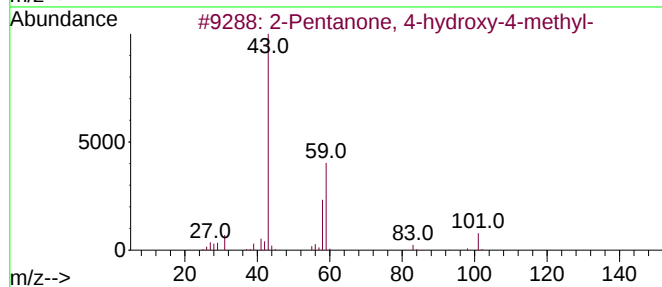
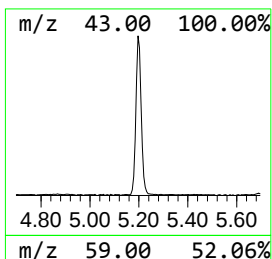
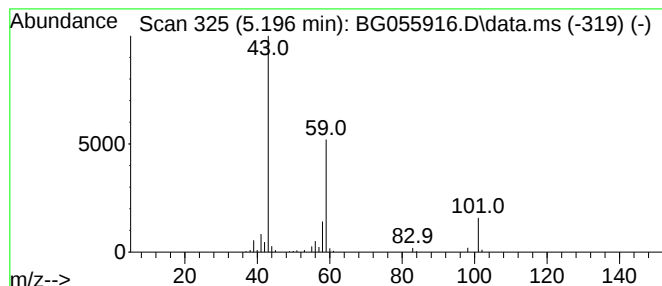
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.196	24.85 ng	158848	1,4-Dichlorobenzene-d4			8.158
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	37
3	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	27
5	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	17



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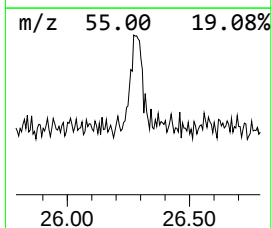
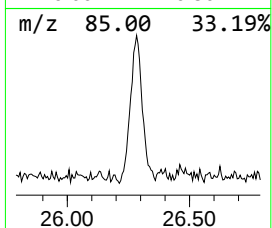
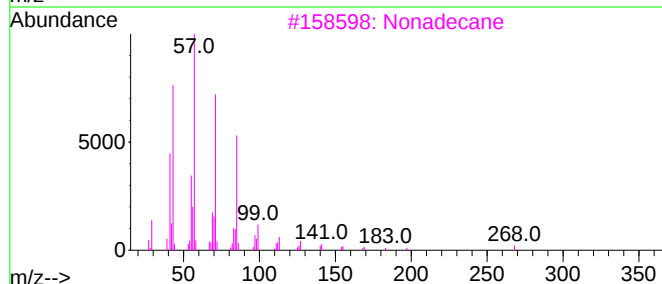
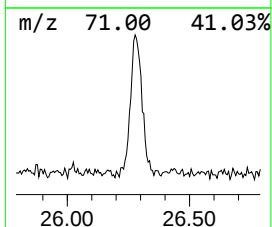
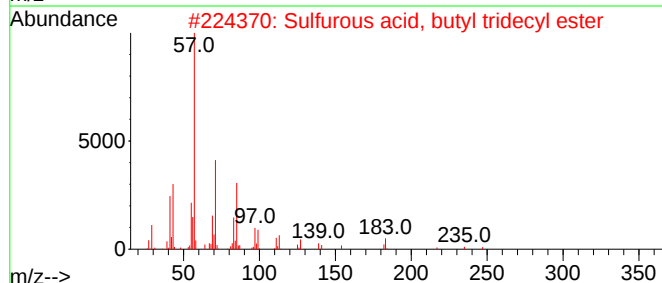
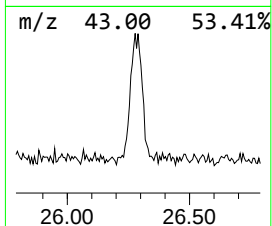
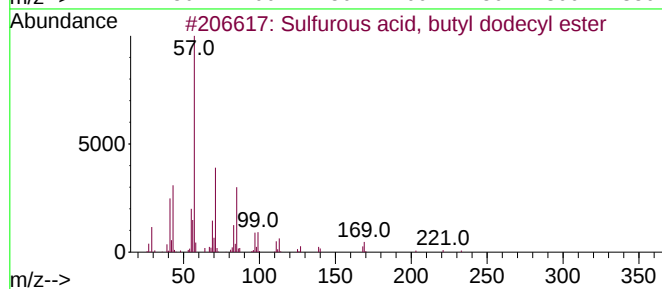
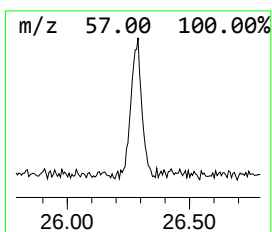
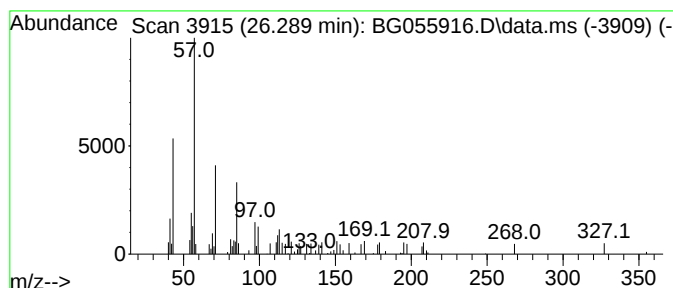
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Peak Number 2 Sulfurous acid, butyl dodec... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.289	2.19 ng	68625	Perylene-d12	25.167

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	80
2			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	72
3			Nonadecane	268	C19H40	000629-92-5	70
4			Eicosane	282	C20H42	000112-95-8	59
5			Dodecane, 3-methyl-	184	C13H28	017312-57-1	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.196	24.9	ng	158848	1	8.158	127862	20.0
Sulfurous acid,...	26.289	2.2	ng	68625	6	25.167	625546	20.0