

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062824\
 Data File : VU059605.D
 Acq On : 28 Jun 2024 08:37
 Operator : MD/SY
 Sample : P3007-15
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 JMRG4

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

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:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU059605.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.354	14	20	37	rBV	105850	121855	22.84%	2.244%
2	1.589	84	93	107	rVB2	73432	112051	21.00%	2.063%
3	1.724	130	135	146	rVB	9266	10866	2.04%	0.200%
4	1.907	183	192	207	rBV	56397	77190	14.47%	1.421%
5	2.557	382	394	410	rVB	101965	166147	31.14%	3.059%
6	2.669	413	429	432	rBV4	5886	13613	2.55%	0.251%
7	2.788	455	466	476	rBV2	4772	7380	1.38%	0.136%
8	2.962	511	520	527	rBV4	2995	5691	1.07%	0.105%
9	3.036	532	543	564	rVB2	9490	20475	3.84%	0.377%
10	4.640	1026	1042	1076	rBV	41103	164821	30.90%	3.035%
11	5.055	1156	1171	1192	rBV	101448	229221	42.97%	4.221%
12	5.718	1357	1377	1405	rBV2	200927	520796	97.63%	9.589%
13	6.242	1528	1540	1568	rBV	166885	320118	60.01%	5.894%
14	6.537	1619	1632	1649	rBV	120893	232379	43.56%	4.279%
15	6.682	1664	1677	1706	rBV	124684	244738	45.88%	4.506%
16	7.560	1936	1950	1974	rBV2	44971	82361	15.44%	1.516%
17	7.891	2041	2053	2066	rBV	238192	416013	77.98%	7.660%
18	7.962	2066	2075	2096	rVB	91163	162260	30.42%	2.988%
19	8.174	2131	2141	2159	rBV2	26458	47962	8.99%	0.883%
20	8.631	2271	2283	2321	rBV	211973	470380	88.17%	8.661%
21	8.785	2324	2331	2343	rVB8	5478	10849	2.03%	0.200%
22	9.412	2514	2526	2545	rBV	253178	422376	79.18%	7.777%
23	10.749	2930	2942	2960	rBV2	100875	161858	30.34%	2.980%
24	11.807	3259	3271	3292	rBV	229210	380848	71.39%	7.012%
25	12.061	3342	3350	3371	rBV7	6112	16705	3.13%	0.308%
26	12.187	3377	3389	3412	rBV	228977	381271	71.47%	7.020%
27	12.524	3488	3494	3504	rVB4	3835	5924	1.11%	0.109%
28	13.000	3634	3642	3651	rBV4	3478	5493	1.03%	0.101%
29	15.685	4469	4477	4488	rVB7	9514	13483	2.53%	0.248%
30	16.759	4802	4811	4824	rBV2	48434	72433	13.58%	1.334%
31	16.878	4837	4848	4871	rBV	344396	533465	100.00%	9.823%

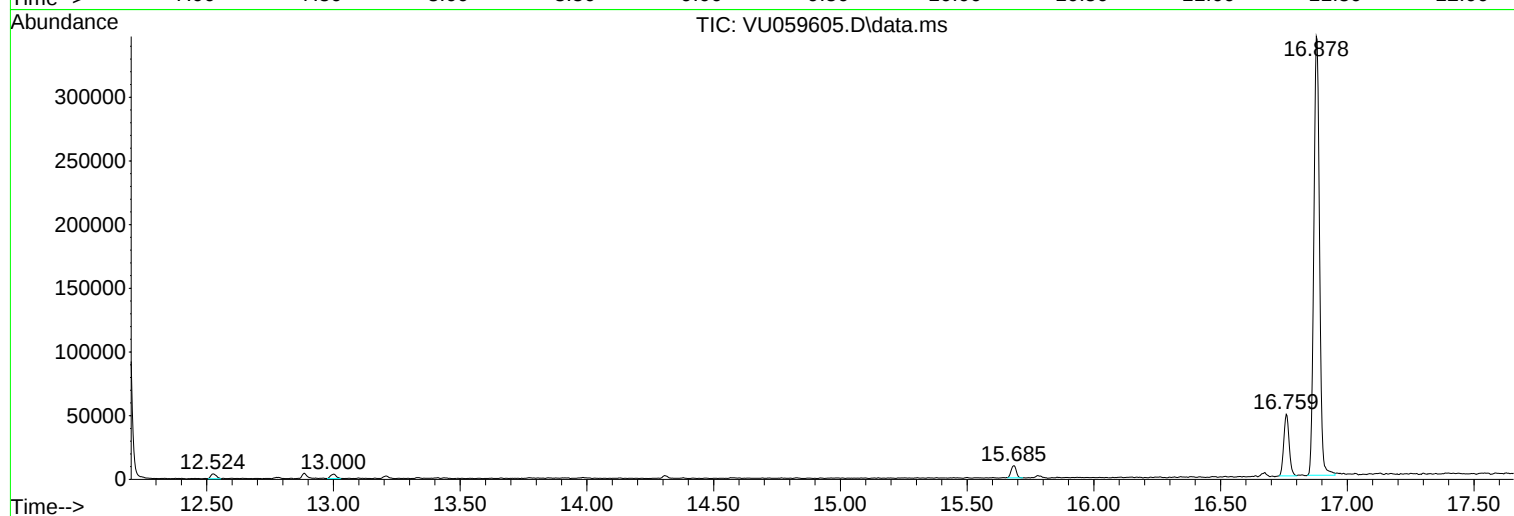
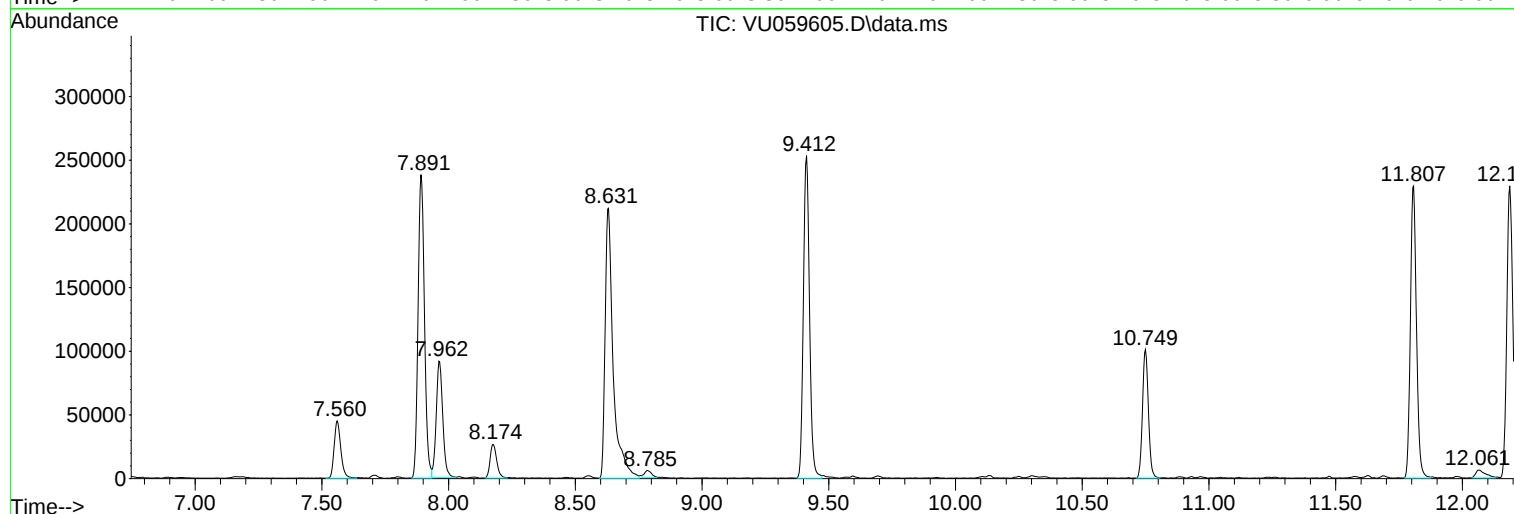
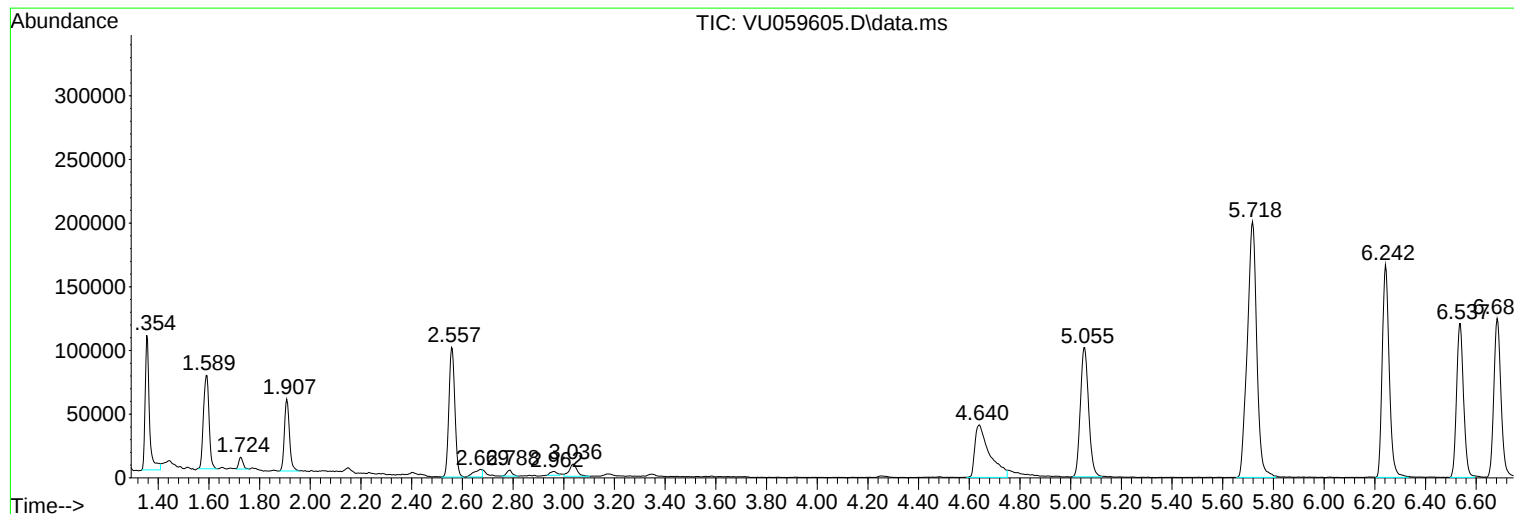
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ClientSampleId :
JMRG4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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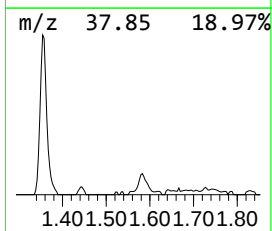
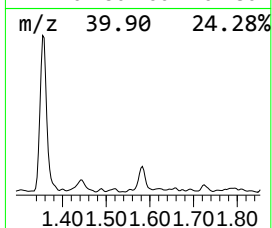
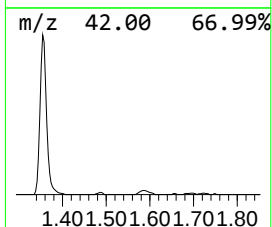
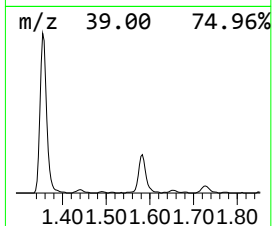
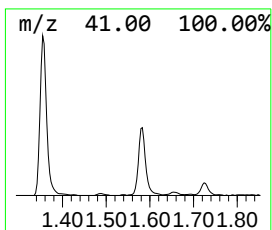
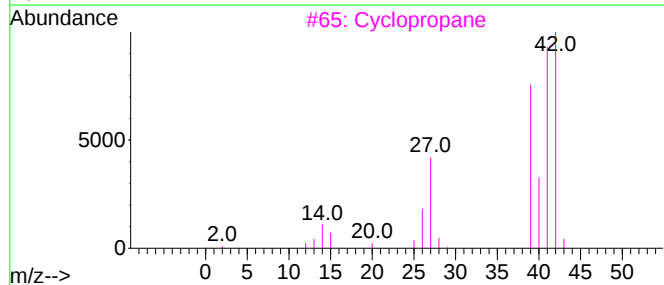
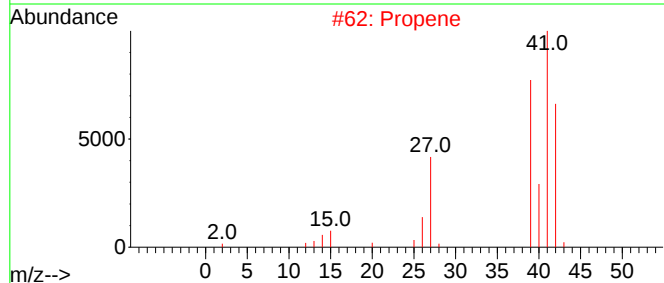
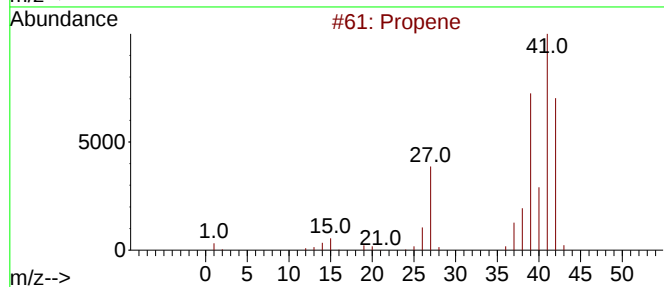
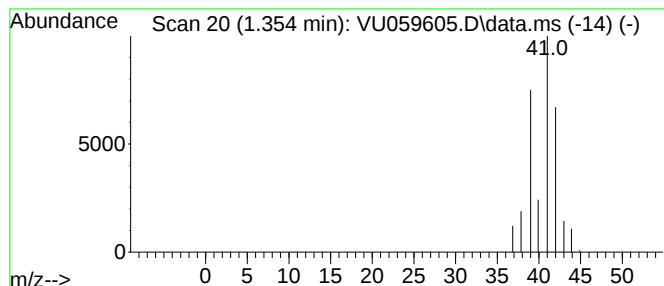
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.354	1.90 ug/L	121855	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Propene	42	C3H6	000115-07-1	56
3			Cyclopropane	42	C3H6	000075-19-4	9
4			Cyclopropane	42	C3H6	000075-19-4	9
5			Cyclopropane	42	C3H6	000075-19-4	9



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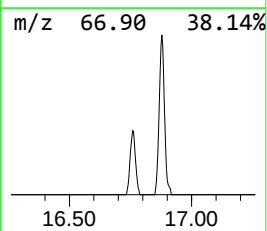
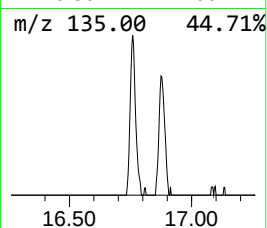
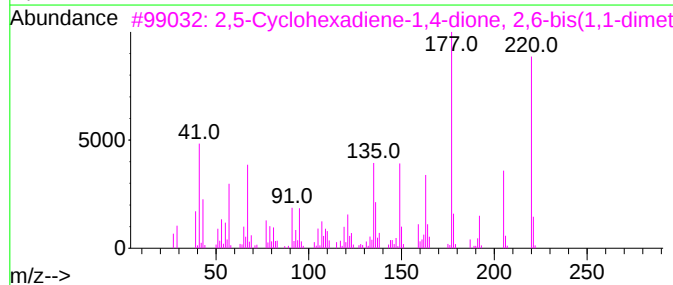
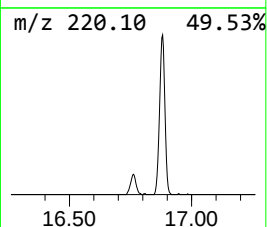
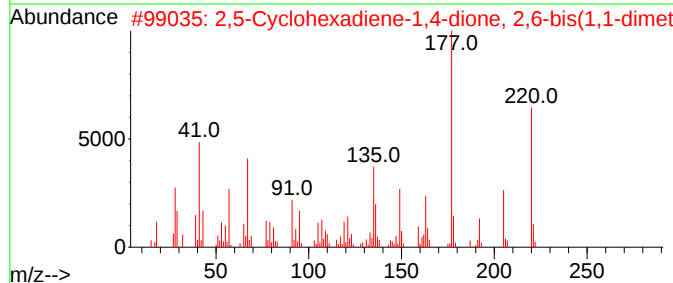
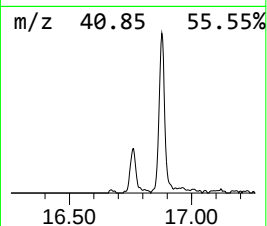
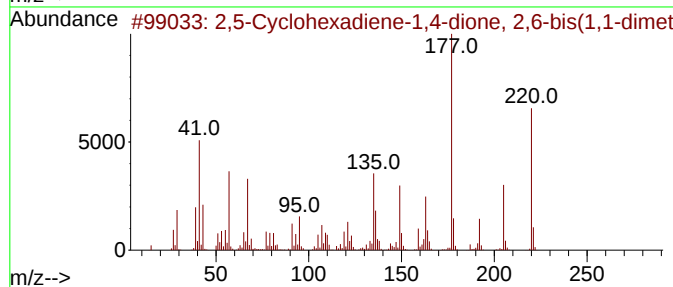
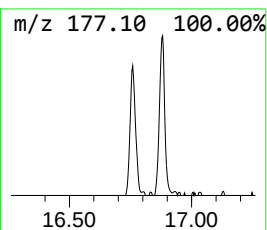
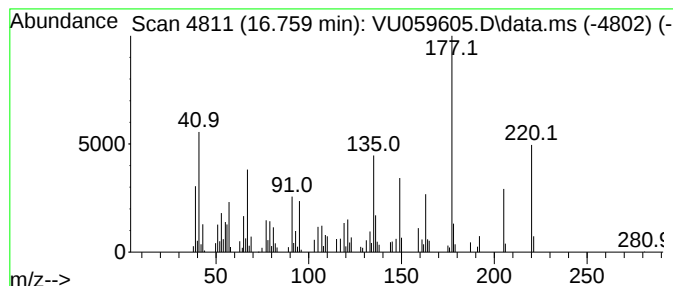
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.759	0.95 ug/L	72433	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	55		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	55		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	55		
5	trans-.beta.-Ionone	192	C13H200	000079-77-6	52		



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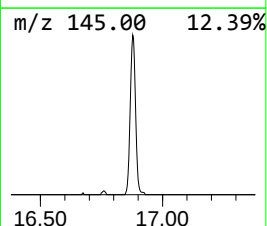
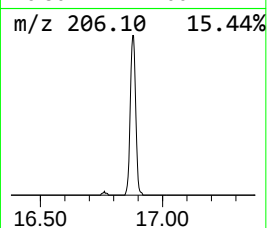
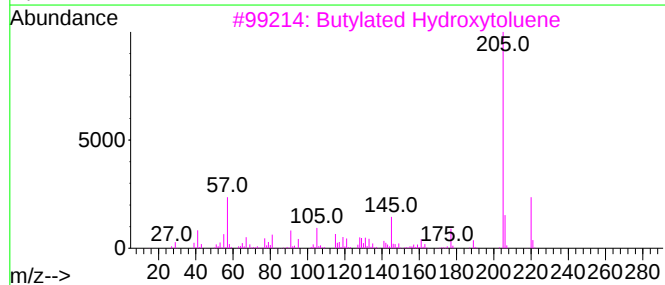
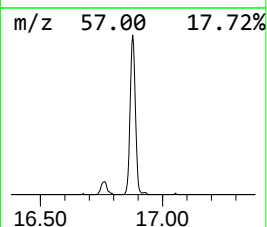
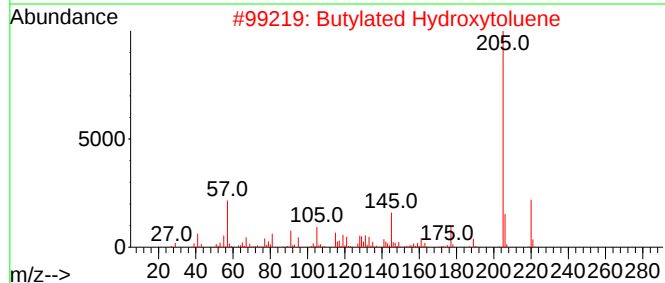
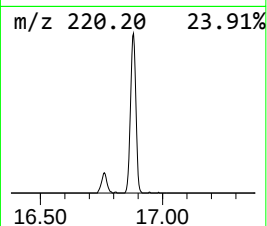
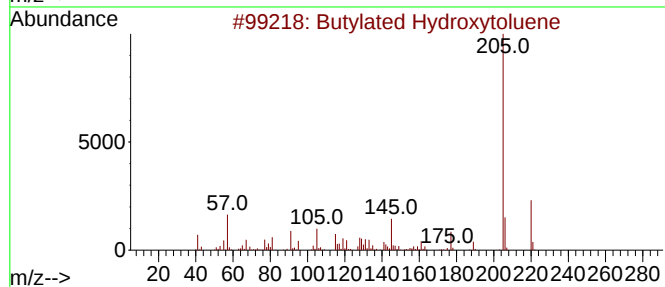
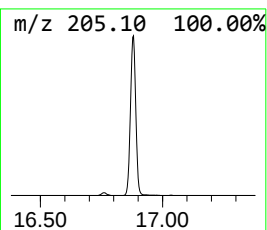
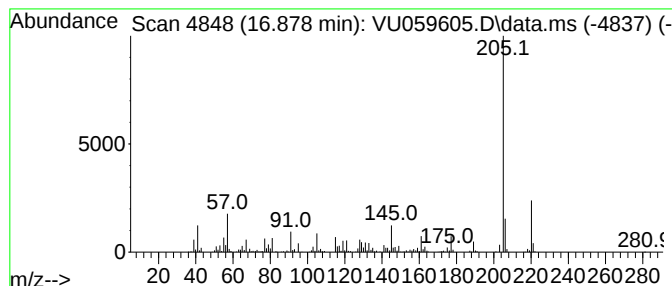
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.878	7.00 ug/L	533465	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
4			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	96
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96



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Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.354	1.9	ug/L	121855	1	6.242	320118	5.0
2,5-Cyclohexadi...	16.759	0.9	ug/L	72433	3	11.807	380848	5.0
Butylated Hydro...	16.878	7.0	ug/L	533465	3	11.807	380848	5.0