LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071723\
Data File : BP016269.D
Acq On : 18 Jul 2023 00:04
Operator : MA/JU
Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A46R9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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_P\Methods\SFAM-EPA-BP071223.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP016269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.281	13	16	23	rVB	28058	42635	0.75%	0.069%
2	3.770	97	99	109	rBV2	54447	152026	2.66%	0.247%
3	3.940	126	128	134	rVB	16122	20224	0.35%	0.033%
4	4.046	142	146	154	rVB	51129	82230	1.44%	0.134%
5	4.446	210	214	224	rBV3	27117	50705	0.89%	0.082%
6	5.469	382	388	390	rBV7	5292	10751	0.19%	0.017%
7	5.816	442	447	454	rBV8	4726	9623	0.17%	0.016%
8	5.981	469	475	482	rVV	135769	269988	4.72%	0.438%
9	6.046	482	486	499	rVB2	38975	124495	2.18%	0.202%
10	6.528	562	568	572	rBV9	4065	7659	0.13%	0.012%
11	6.605	576	581	594	rBV2	38689	104403	1.83%	0.170%
12	7.193	672	681	693	rBV5	61919	230912	4.04%	0.375%
13	7.293	693	698	729	rVV	371757	1050701	18.38%	1.706%
14	7.516	729	736	760	rVV	309574	897480	15.70%	1.457%
15	7.681	762	764	772	rVB9	6608	12782	0.22%	0.021%
16	7.963	805	812	821	rBV	461067	1139624	19.93%	1.850%
17	8.234	854	858	864	rVB9	5684	11157	0.20%	0.018%
18	8.328	868	874	879	rVV8	9870	22510	0.39%	0.037%
19	8.652	925	929	935	rBV9	8667	22667	0.40%	0.037%
20	8.722	935	941	958	rVV3	201877	761228	13.31%	1.236%
21	8.840	958	961	980	rVB	51520	131373	2.30%	0.213%
22	9.081	995	1002	1009	rBV	264751	523891	9.16%	0.851%
23	9.157	1009	1015	1037	rVB	469484	1380215	24.14%	2.241%
24	9.310	1037	1041	1043	rBV4	14750	21496	0.38%	0.035%
25	9.463	1065	1067	1071	rVB5	7362	9122	0.16%	0.015%
26	9.893	1133	1140	1160	rBV2	281385	944870	16.53%	1.534%
27	10.040	1160	1165	1184	rVV	91036	238058	4.16%	0.386%
28	10.175	1184	1188	1192	rVB7	11185	18791	0.33%	0.031%
29	10.287	1201	1207	1223	rBV	82719	233576	4.09%	0.379%
30	10.404	1223	1227	1230	rBV6	5328	8047	0.14%	0.013%
31	10.481	1233	1240	1264	rBV2	277099	1348171	23.58%	2.189%
32	10.775	1284	1290	1312	rVB	971325	2232329	39.05%	3.624%
33	10.981	1318	1325	1336	rBV	270666	955325	16.71%	1.551%
34	11.069	1336	1340	1358	rVB2	138236	397201	6.95%	0.645%
35	11.581	1425	1427	1439	rVB2	6581	18728	0.33%	0.030%
36	11.804	1462	1465	1468	rBV5	5648	6845	0.12%	0.011%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071723\
Data File : BP016269.D
Acq On : 18 Jul 2023 00:04
Operator : MA/JU
Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A46R9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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_P\Methods\SFAM-EPA-BP071223.MA.M
Title : SVOA CALIBRATION

37	11.940	1479	1488	1497	rBV4	21718	54601	0.96%	0.089%
38	12.169	1522	1527	1532	rBV7	8002	16468	0.29%	0.027%
39	12.446	1568	1574	1580	rBV7	10234	23736	0.42%	0.039%
40	12.510	1580	1585	1597	rVB	25506	53409	0.93%	0.087%
41	12.951	1654	1660	1682	rVV	61467	233366	4.08%	0.379%
42	13.157	1690	1695	1696	rBV5	5752	6591	0.12%	0.011%
43	13.204	1696	1703	1718	rVB	167718	291614	5.10%	0.473%
44	13.357	1724	1729	1733	rVB8	3916	7243	0.13%	0.012%
45	13.487	1747	1751	1757	rBV2	19723	36382	0.64%	0.059%
46	13.610	1768	1772	1777	rVB8	3771	6659	0.12%	0.011%
47	13.675	1777	1783	1784	rBV	37040	48632	0.85%	0.079%
48	13.845	1808	1812	1815	rBV5	9044	13684	0.24%	0.022%
49	14.034	1836	1844	1855	rBV	1242074	2558510	44.75%	4.154%
50	14.310	1883	1891	1908	rBV	1851081	3116274	54.51%	5.059%
51	14.475	1917	1919	1930	rVB	8834	16129	0.28%	0.026%
52	14.610	1935	1942	1953	rBV	1903209	3032637	53.04%	4.924%
53	15.163	2026	2036	2039	rBV	11205	34922	0.61%	0.057%
54	15.292	2055	2058	2064	rVB2	13777	23966	0.42%	0.039%
55	15.381	2069	2073	2076	rBV2	11131	15646	0.27%	0.025%
56	15.457	2082	2086	2094	rVB	22768	36318	0.64%	0.059%
57	15.522	2094	2097	2101	rVB6	5447	7152	0.13%	0.012%
58	15.616	2106	2113	2136	rBV	1805347	4066900	71.13%	6.603%
59	15.845	2146	2152	2153	rBV2	94874	119442	2.09%	0.194%
60	15.981	2173	2175	2180	rVB5	16285	17421	0.30%	0.028%
61	16.022	2180	2182	2190	rVB5	15236	26047	0.46%	0.042%
62	16.234	2215	2218	2224	rVB8	6689	9996	0.17%	0.016%
63	16.310	2229	2231	2235	rVB5	5785	6311	0.11%	0.010%
64	16.563	2268	2274	2275	rBV6	5989	8848	0.15%	0.014%
65	16.686	2288	2295	2299	rBV8	6213	15107	0.26%	0.025%
66	16.798	2307	2314	2315	rBV6	7130	11669	0.20%	0.019%
67	17.186	2376	2380	2384	rVB6	6630	10686	0.19%	0.017%
68	17.375	2406	2412	2424	rBV	2418459	3734340	65.32%	6.063%
69	17.486	2425	2431	2457	rVB	1986562	4442941	77.71%	7.213%
70	17.833	2488	2490	2499	rBV10	6407	10172	0.18%	0.017%
71	18.010	2514	2520	2535	rBV	2296823	2762498	48.32%	4.485%
72	18.257	2558	2562	2566	rBV7	15986	29648	0.52%	0.048%
73	18.333	2571	2575	2581	rVV5	10387	22904	0.40%	0.037%
74	18.439	2589	2593	2598	rBV3	23813	40845	0.71%	0.066%
75	18.480	2598	2600	2603	rVB3	14790	16264	0.28%	0.026%
76	19.298	2735	2739	2743	rVB3	35691	48148	0.84%	0.078%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071723\
Data File : BP016269.D
Acq On : 18 Jul 2023 00:04
Operator : MA/JU
Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46R9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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_P\Methods\SFAM-EPA-BP071223.MA.M
Title : SVOA CALIBRATION

77	19.375	2748	2752	2760	rBV	31057	58850	1.03%	0.096%
78	19.598	2786	2790	2796	rBV	77928	108829	1.90%	0.177%
79	19.716	2804	2810	2835	rBV	2859376	5717191	100.00%	9.282%
80	21.480	3104	3110	3128	rBV	2040004	4620348	80.82%	7.501%
81	22.551	3287	3292	3309	rVB	2120559	3172907	55.50%	5.151%
82	23.792	3497	3503	3520	rVB2	2305122	5206819	91.07%	8.453%
83	23.968	3526	3533	3556	rVB	1350513	4182792	73.16%	6.791%

Sum of corrected areas: 61593700

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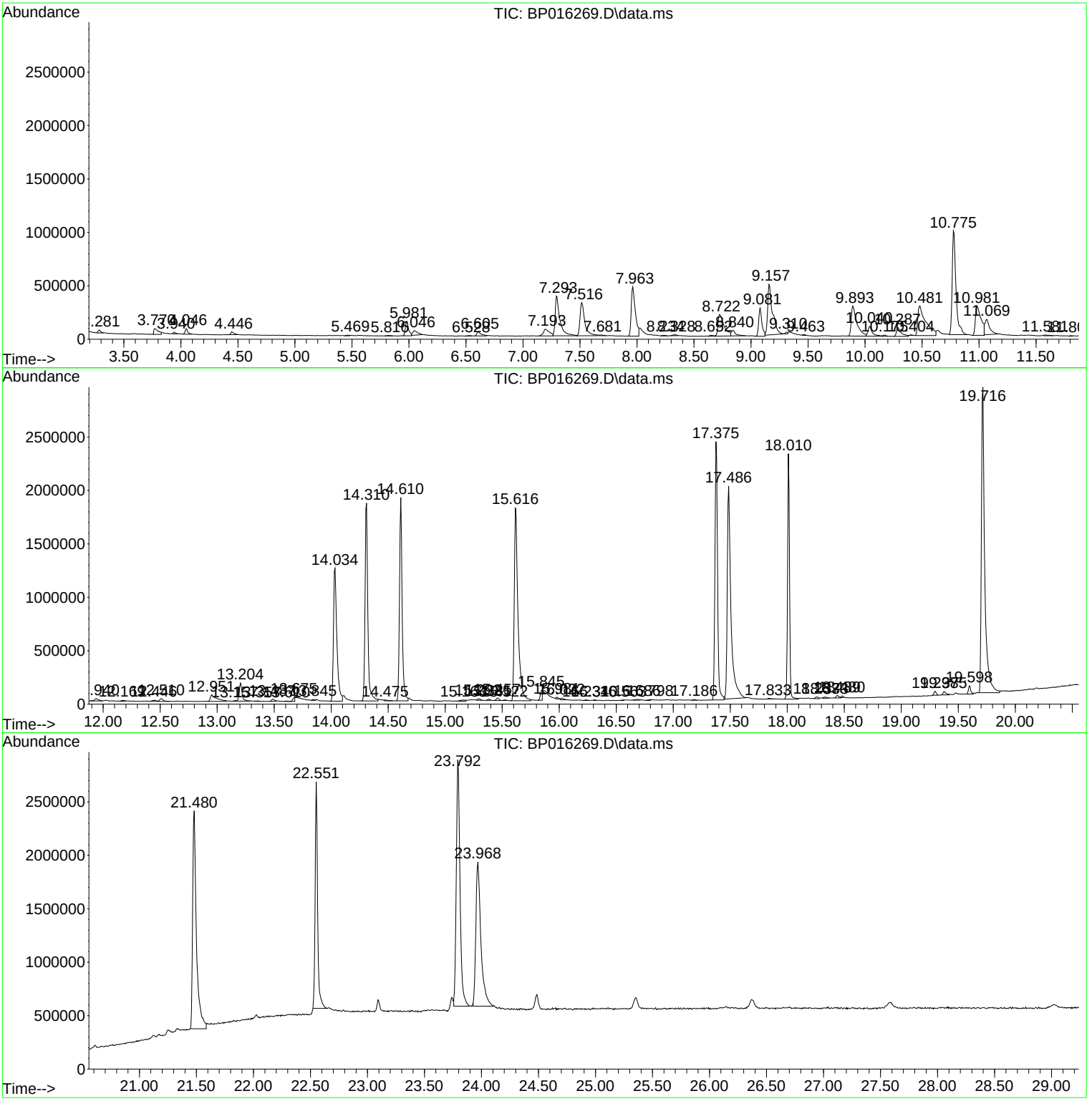
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46R9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071723\
Data File : BP016269.D
Acq On : 18 Jul 2023 00:04
Operator : MA/JU
Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46R9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

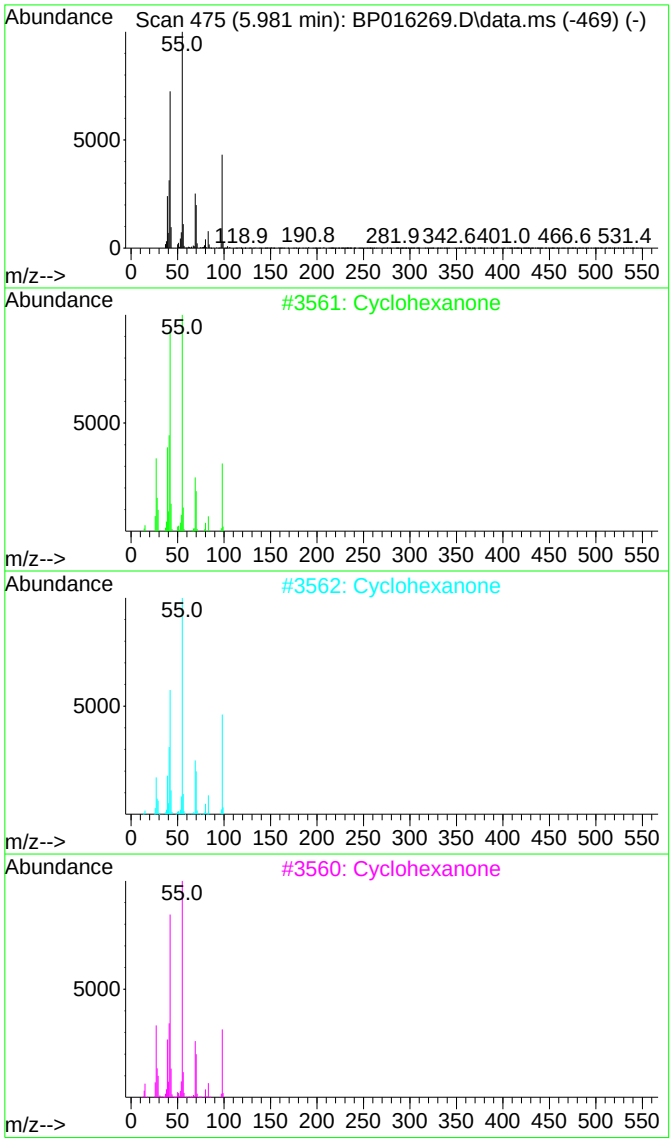
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

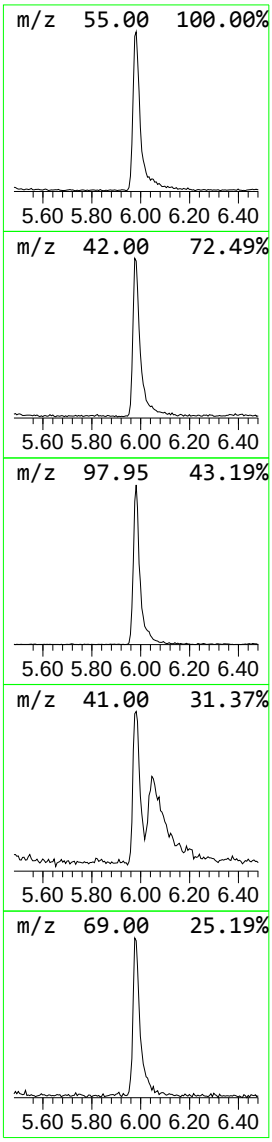
****

Peak Number 1 Cyclohexanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.981	4.74 ng/ul	269988	1,4-Dichlorobenzene-d4	7.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	91
2	Cyclohexanone	98	C6H10O	000108-94-1	91
3	Cyclohexanone	98	C6H10O	000108-94-1	91
4	Cyclohexanone	98	C6H10O	000108-94-1	90
5	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071723\
Data File : BP016269.D
Acq On : 18 Jul 2023 00:04
Operator : MA/JU
Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46R9

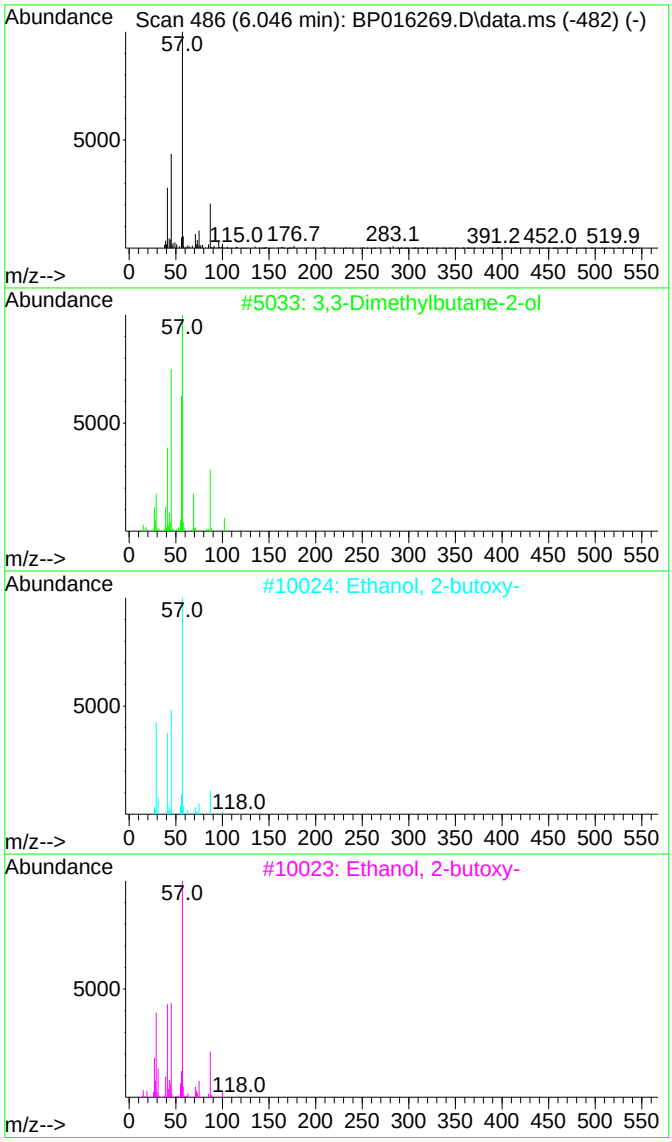
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

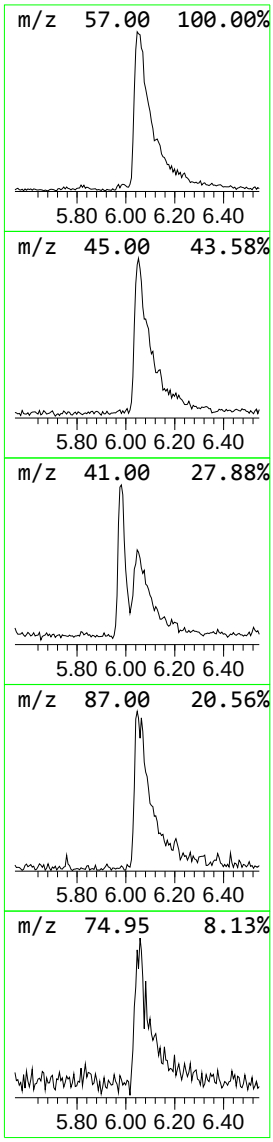
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3,3-Dimethylbutane-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.046	2.18 ng/ul	124495	1,4-Dichlorobenzene-d4	7.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	64
2	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	64
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	56
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071723\
Data File : BP016269.D
Acq On : 18 Jul 2023 00:04
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Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46R9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

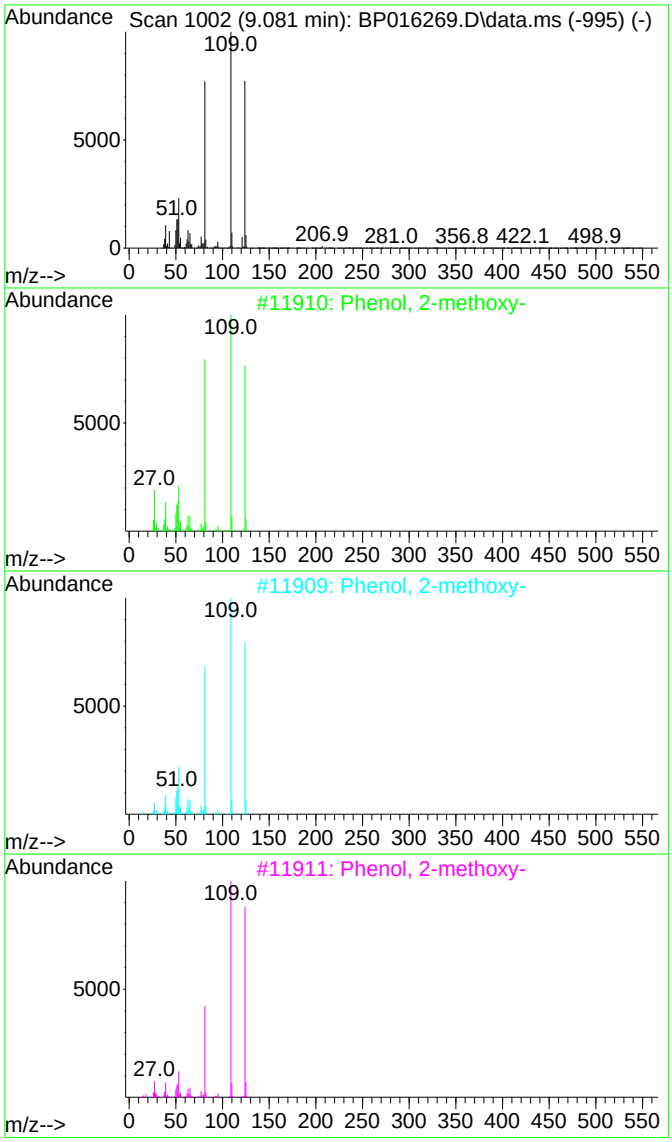
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

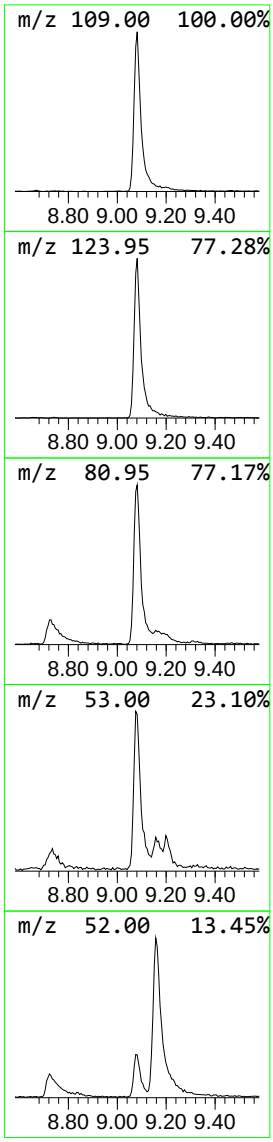
****

Peak Number 4 Phenol, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.081	9.19 ng/ul	523891	1,4-Dichlorobenzene-d4	7.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	97
2	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	96
3	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	95
4	Mequinol	124	C7H8O2	000150-76-5	91
5	Mequinol	124	C7H8O2	000150-76-5	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071723\
Data File : BP016269.D
Acq On : 18 Jul 2023 00:04
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Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46R9

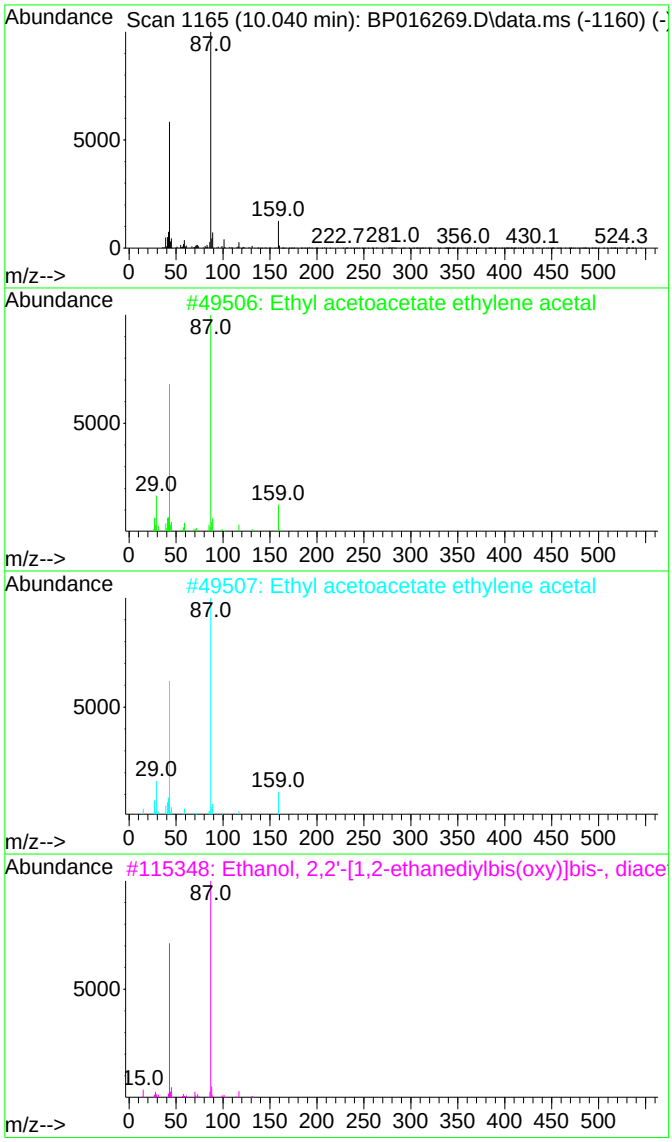
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

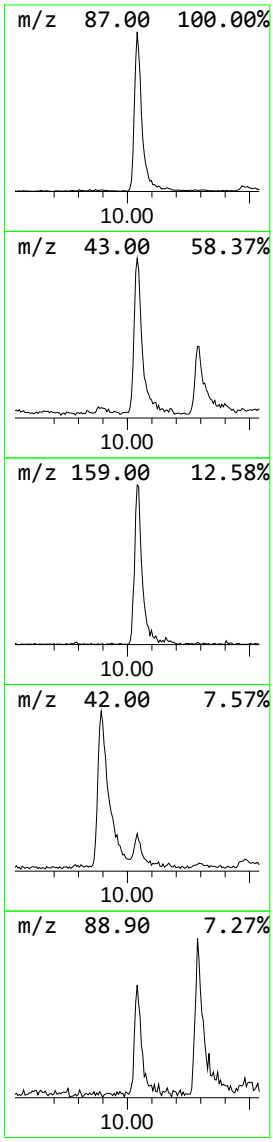
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethyl acetoacetate ethylene... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.040	2.13 ng/ul	238058	Naphthalene-d8	10.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl acetoacetate ethylene acetal	174	C8H14O4	006413-10-1	80
2	Ethyl acetoacetate ethylene acetal	174	C8H14O4	006413-10-1	72
3	Ethanol, 2,2'-[1,2-ethanediylbis...	234	C10H18O6	000111-21-7	53
4	1,3-Dioxolane-2-propanoic acid, ...	188	C9H16O4	000941-43-5	45
5	Tetraethylene glycol, diacetate	278	C12H22O7	022790-12-1	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071723\
Data File : BP016269.D
Acq On : 18 Jul 2023 00:04
Operator : MA/JU
Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46R9

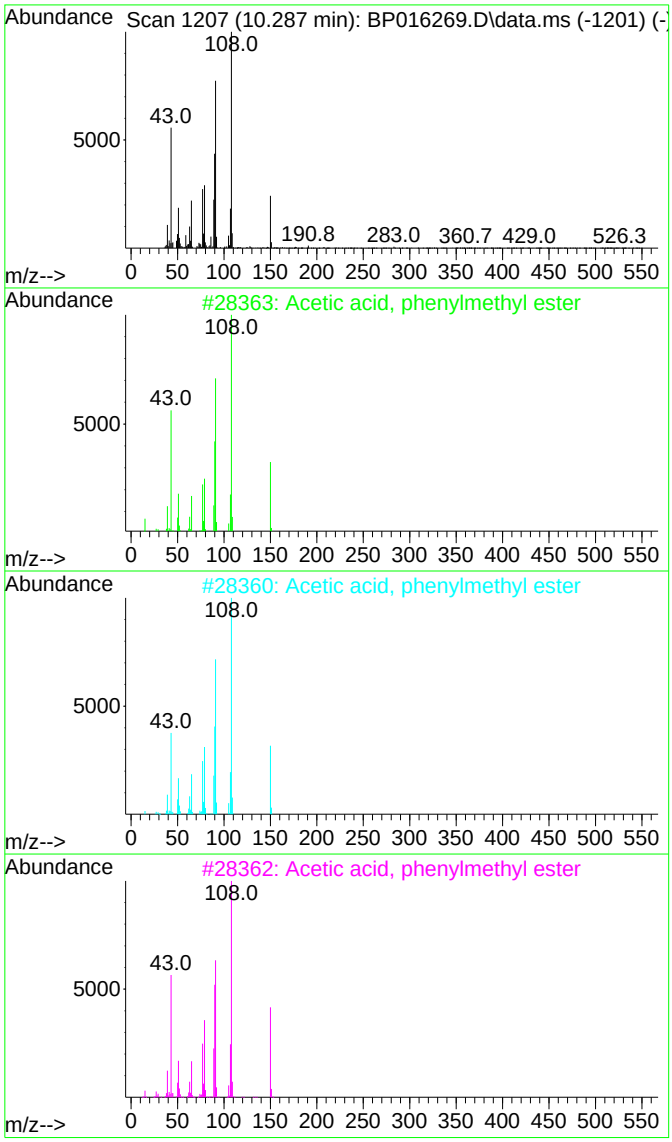
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

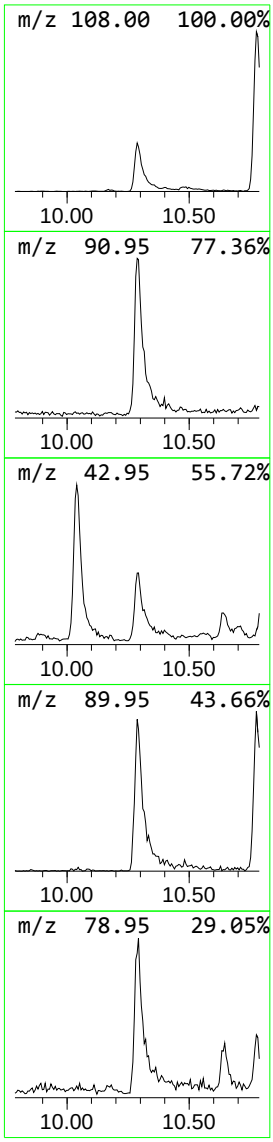
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Acetic acid, phenylmethyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.287	2.09 ng/ul	233576	Naphthalene-d8	10.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	97
2	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	96
3	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	93
4	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	81
5	Formic acid, phenylmethyl ester	136	C8H8O2	000104-57-4	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071723\
Data File : BP016269.D
Acq On : 18 Jul 2023 00:04
Operator : MA/JU
Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46R9

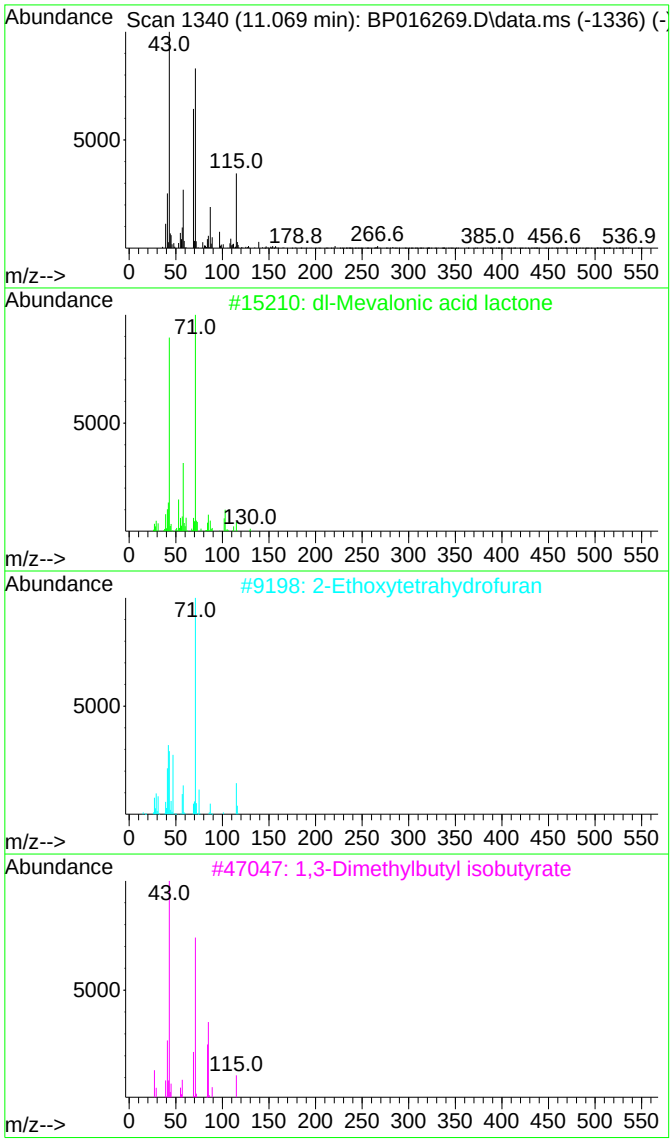
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

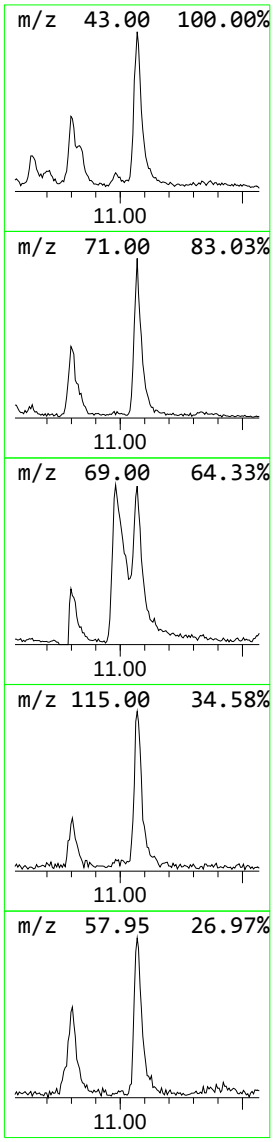
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 dl-Mevalonic acid lactone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.069	3.56 ng/ul	397201	Naphthalene-d8	10.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	50
2	2-Ethoxytetrahydrofuran	116	C6H12O2	013436-46-9	43
3	1,3-Dimethylbutyl isobutyrate	172	C10H20O2	1000429-31-6	43
4	Butyric acid, 4-pentadecyl ester	298	C19H38O2	1000280-57-4	43
5	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	40





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Acq On : 18 Jul 2023 00:04
Operator : MA/JU
Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46R9

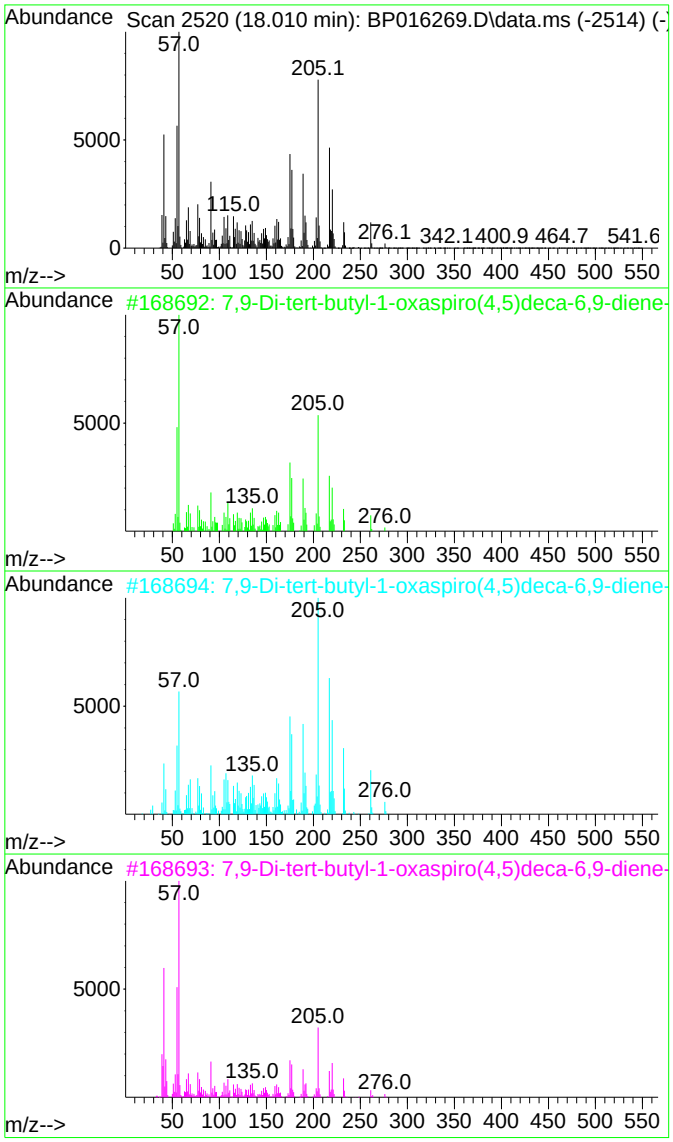
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

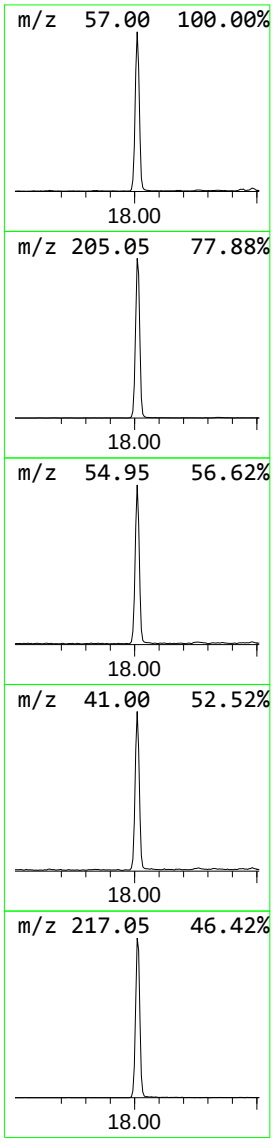
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.010	14.80 ng/ul	2762500	Phenanthrene-d10	17.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	83
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	60
4	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	55
5	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071723\
Data File : BP016269.D
Acq On : 18 Jul 2023 00:04
Operator : MA/JU
Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46R9

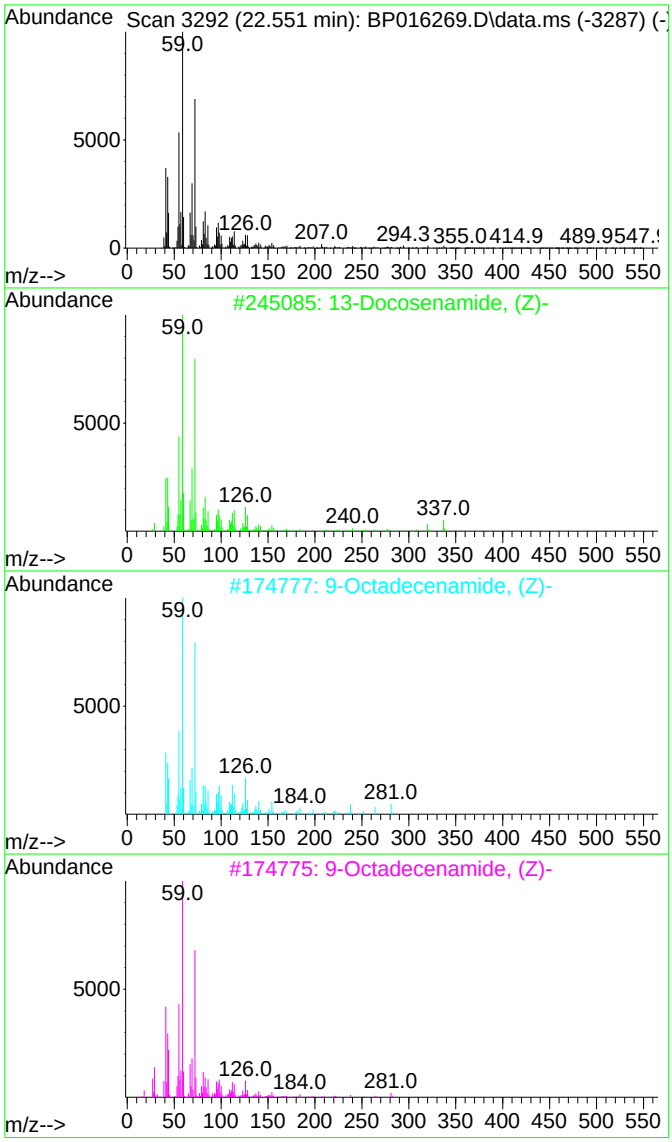
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

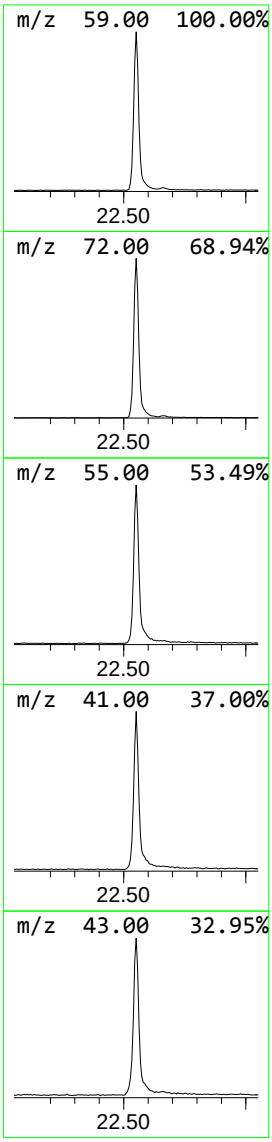
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.551	13.73 ng/ul	3172910	Chrysene-d12	21.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
4	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071723\
Data File : BP016269.D
Acq On : 18 Jul 2023 00:04
Operator : MA/JU
Sample : 03423-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A46R9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071223.MA.M
Quant Title : SVOA CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclohexanone	5.981	4.7	ng/ul	269988	1	7.963	1139620	20.0
3,3-Dimethylbut...	6.046	2.2	ng/ul	124495	1	7.963	1139620	20.0
Phenol, 2-methoxy-	9.081	9.2	ng/ul	523891	1	7.963	1139620	20.0
Ethyl acetoacet...	10.040	2.1	ng/ul	238058	2	10.775	2232330	20.0
Acetic acid, ph...	10.287	2.1	ng/ul	233576	2	10.775	2232330	20.0
dl-Mevalonic ac...	11.069	3.6	ng/ul	397201	2	10.775	2232330	20.0
7,9-Di-tert-but...	18.010	14.8	ng/ul	2762500	4	17.375	3734340	20.0
13-Docosenamide...	22.551	13.7	ng/ul	3172910	5	21.480	4620350	20.0